

Supporting Information for

**Copper-catalyzed annulation reaction of diazo esters with propargyl  
amines for the synthesis of 2,5-dihydropyrroles**

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## Table of Contents

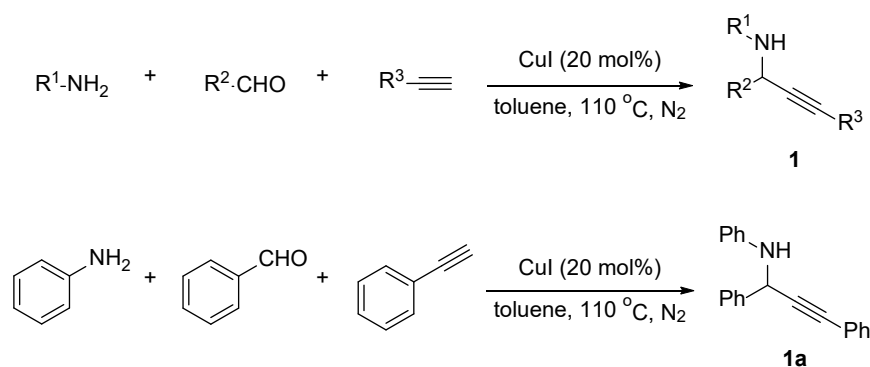
1. General considerations.....	3
2. General procedure for starting materials.....	3
2.1 Preparation of propargyl amines ( <b>1</b> ) <sup>[9]</sup> .....	3
2.2 Preparation of $\alpha$ -diazo esters ( <b>2</b> ) <sup>[10]</sup> .....	4
3. General procedure for the synthesis of multisubstituted 2,5-dihydropyrroles ( <b>3</b> ).....	5
3.1 Experimental procedure with diazo esters as substrates .....	5
3.2 Experimental procedure with <i>N</i> -tosylhydrazone as a substrate.....	5
4. General procedure for synthetic applications .....	6
4.1 Procedure for gram scale reaction.....	6
4.2 Typical procedure for the synthesis of <b>5</b> <sup>[11]</sup> .....	6
4.3 Typical procedure for the synthesis of <b>6</b> <sup>[12]</sup> .....	7
5. Control experiments.....	7
5.1 Radical trap experiment .....	7
5.2 Steric hindrance competition experiments .....	8
5.3 Deuterium isotope exchange experiments.....	9
5.4 With one equivalent base as additive .....	11
5.5 Online detection of pH experiments.....	12
5.6 Intermediate trap experiments.....	12
6. DFT studies .....	15
6.1 Computational methodology .....	15
6.2 Computed Energies for all the structures .....	16
6.3 CYLview Structures and cartesian coordinates of the optimized geometries .....	17
7. X-Ray crystallographic studies .....	62
8. Analytical data .....	64
9. Copies of NMR spectra for compounds.....	82
10. Supplementary Reference .....	126

## 1. General considerations

$^1\text{H}$  and  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra were recorded on a Bruker DRX-400 spectrometer and Bruker AVANCE NEO-500 spectrometer. All chemical shift values refer to  $\delta_{\text{TMS}} = 0.00$  ppm,  $\text{CDCl}_3$  ( $\delta(^1\text{H})$ , 7.26 ppm;  $\delta(^{13}\text{C})$ , 77.16 ppm). The HRMS (EI) analysis was obtained on the Agilent electrospray ionization-time of flight (ESI-TOF) mass spectrometer. Analytical TLC plates, Sigma-Aldrich silica gel 60F200 were viewed by UV light (254 nm). Column chromatographic purifications were performed on SDZF silica gel 160. The valence states of elements in the copper catalyst were determined by X-ray photoelectron spectroscopy (XPS) using Thermo K-Alpha XPS. Melting points were measured with a melting point instrument without correction. All the chemical reagents were purchased from commercial sources and used as received unless otherwise indicated. Compounds **1a**,<sup>1</sup> **1p**,<sup>2</sup> **1q**,<sup>2</sup> **1r**,<sup>3</sup> **1s**,<sup>4</sup> **1t**,<sup>2</sup> **1v**,<sup>5</sup> **1w**,<sup>5</sup> **1x**,<sup>6</sup> **1y**,<sup>1</sup> **1z**,<sup>1</sup> **1z1**,<sup>2</sup> **1z2**,<sup>4</sup> **1z3**,<sup>1</sup> **1z4**,<sup>7</sup> **1z5**<sup>8</sup> are known and their spectroscopic feature is in good agreement with that reported in the literature.

## 2. General procedure for starting materials

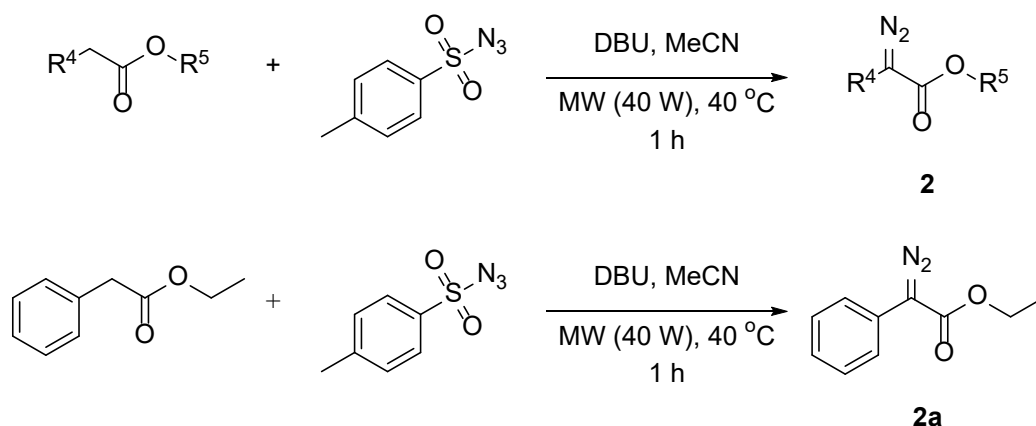
### 2.1 Preparation of propargyl amines (**1**)<sup>[9]</sup>



**A typical procedure for the synthesis of propargyl amines – Synthesis of 1a:** Under a  $\text{N}_2$  atmosphere, a mixture of benzaldehyde (1.06 g, 10 mmol), aniline (1.21 g, 13 mmol), phenylacetylene (1.33 g, 13 mmol), and  $\text{CuI}$  (0.38 g, 2 mmol) in toluene (10 mL) was stirred at  $110\text{ }^\circ\text{C}$  for 12 h with monitoring by TLC. After cooling to ambient

temperature, the reaction mixture was filtered with celite and solvent was evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (60-90 °C)/AcOEt = 50:1, v/v) to afford the corresponding *N*-phenyl- $\alpha$ -(2-phenylethynyl)benzenemethanamine **1a** (2.00 g, 71%) as a yellow solid.

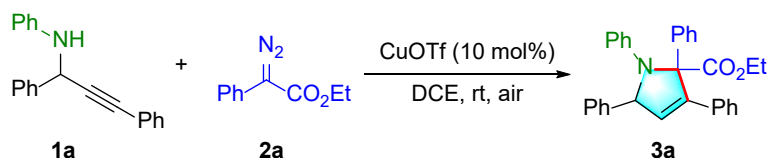
## 2.2 Preparation of $\alpha$ -diazo esters (**2**)<sup>[10]</sup>



**A typical procedure for the synthesis of  $\alpha$ -diazo esters – Synthesis of **2a**:** DBU (2.24 mL, 15 mmol) was added slowly to a stirred solution of methyl 2-phenylacetate (1.41 mL, 10 mmol) and tosylazide (2.42 mL, 11 mmol) in the CH<sub>3</sub>CN (20 mL) at 0 °C. After that, it was placed in microwave reactor that was heated to 40 °C (400 W, monitored by IR temperature sensor) and maintained at this temperature for 1 h. After cooling to room temperature, the reaction mixture was quenched with saturated aqueous solution of NH<sub>4</sub>Cl (5 mL), extracted with CH<sub>2</sub>Cl<sub>2</sub> (3×30 mL), washed with brine (3×10 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, and concentrated under reduced pressure to form the  $\alpha$ -diazo ester product. The residue was purified by flash chromatography (eluent: petroleum ether (60-90 °C)/EtOAc, 100:1) to afford the corresponding methyl-2-diazo-2-phenylacetate **2a** (1.49 g, 85%) as a yellow oil.

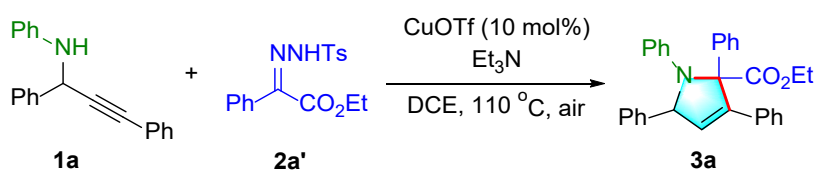
### 3. General procedure for the synthesis of multisubstituted 2,5-dihydropyrroles (3)

#### 3.1 Experimental procedure with diazo esters as substrates



A typical general procedure for the synthesis of *multisubstituted 2,5-dihydropyrroles (3)* – *Synthesis of 3a*: Under an air atmosphere, ethyl 2-diazo-2-phenylacetate **2a** (143 mg, 0.75 mmol in 1 mL of DCE) was added slowly to a mixture of propargyl amine **1a** (142 mg, 0.5 mmol) and CuOTf (11 mg, 0.05 mmol) in 4 mL DCE. Then, the mixture was stirred at room temperature for 1 h. After **1a** was completely consumed by TLC monitoring on silica gel, all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (60-90 °C)/EtOAc, 20:1) to afford the corresponding **3a** (145 mg, 65%) as a white solid.

#### 3.2 Experimental procedure with *N*-tosylhydrazone as a substrate

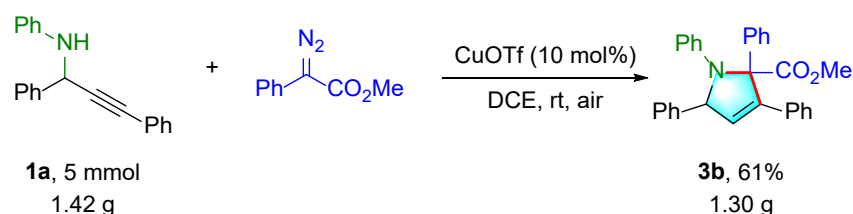


A typical general procedure for the synthesis of *multisubstituted 2,5-dihydropyrroles (3)* – *Synthesis of 3a*: Under an air atmosphere, a mixture of *N*-tosylhydrazone **2a'** (0.75 mmol in 1 mL of DCE) was added slowly the mixture of propargyl amine **1a** (84 mg, 0.5 mmol), and Et<sub>3</sub>N (60 mg, 0.75 mmol) in 4 mL DCE. The reaction mixture was stirred at 110 °C for 3 h. Then, the resultant mixture was cooled to ambient temperature and all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether

(60-90 °C)/EtOAc, 20:1) to afford the corresponding **3a** (29 mg, 13%) as a white solid.

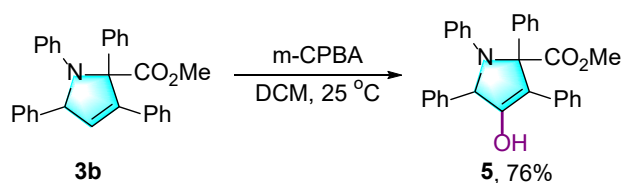
## 4. General procedure for synthetic applications

### 4.1 Procedure for gram scale reaction



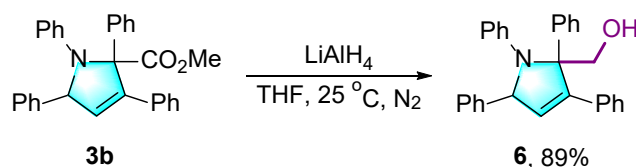
Under an air atmosphere, methyl 2-diazo-2-phenylacetate **2b** (1.32 g, 7.5 mmol in 5 mL of DCE) was added slowly to a mixture of propargyl amine **1a** (1.40 g, 5 mmol) and CuOTf (106 mg, 0.5 mmol) in 15 mL DCE. Then, the mixture was stirred at room temperature for 3 h. After **1a** was completely consumed by TLC monitoring on silica gel, all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (60-90 °C)/EtOAc, 20:1) to afford the corresponding **3b** (1.30 g, 61%) as a white solid.

### 4.2 Typical procedure for the synthesis of **5**<sup>[11]</sup>



Under an air atmosphere, a mixture of dihydropyrrole **3b** (216 mg, 0.5 mmol), and m-CPBA (129 mg, 0.75 mmol) in DCM (5 mL) was stirred at room temperature for 3 h. When TLC monitoring on silica gel indicated complete consumption of dihydropyrrole **3b**, all the volatiles were evaporated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: petroleum ether (60-90 °C)/AcOEt = 20:1, v/v), affording **5** (170 mg, 76%) as a white solid.

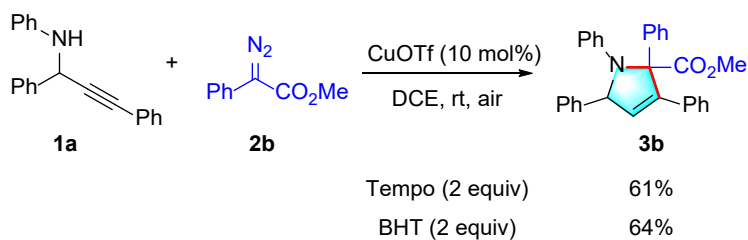
### 4.3 Typical procedure for the synthesis of **6**<sup>[12]</sup>



Under a N<sub>2</sub> atmosphere, lithium aluminium hydride (5 mL, 1M in THF) was added slowly to dihydropyrrole **3b** (216 mg, 0.5 mmol) in 5 mL of THF at 0 °C. Then, the mixture was slowly warmed to room temperature till the completion (2 h) of reaction as monitored by TLC. It was then cooled to 0 °C, and 10 mL of water was added successively. Then, reaction mixture was allowed to stir for 0.5 h, filtered through celite and washed with ethyl acetate, dried over anhydrous sodium sulfate, concentrated and purified by silica gel column chromatography (eluent: petroleum ether (60-90 °C)/AcOEt = 20:1, v/v), affording **6** (179 mg, 89%) as a white solid.

## 5. Control experiments

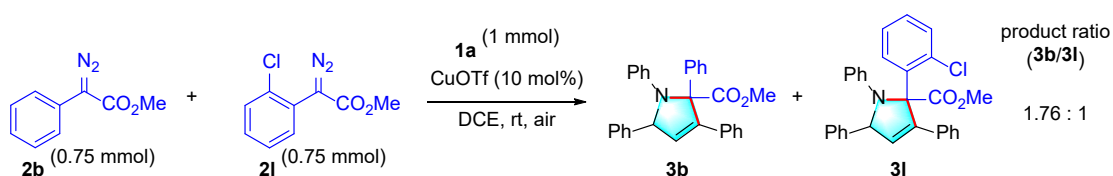
### 5.1 Radical trap experiment



**Experiment procedure with TEMPO as a radical inhibitor:** Under an air atmosphere, methyl 2-diazo-2-phenylacetate **2b** (132 mg, 0.75 mmol in 1 mL of DCE) was added slowly to a mixture of propargyl amine **1a** (142 mg, 0.5 mmol), CuOTf (11 mg, 0.05 mmol), and tempo (156 mg, 1 mmol) in 4 mL DCE. Then, the mixture was stirred at room temperature for 1 h. After the reaction was completely finished, all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (60-90 °C)/EtOAc, 20:1) to afford the corresponding **3b** (132 mg, 61%) as a white solid.

**Experiment procedure with BHT as a radical inhibitor:** Under an air atmosphere, methyl 2-diazo-2-phenylacetate **2b** (132 mg, 0.75 mmol in 1 mL of DCE) was added slowly to a mixture of propargyl amine **1a** (142 mg, 0.5 mmol), CuOTf (11 mg, 0.05 mmol), and BHT (220 mg, 1 mmol) in 4 mL DCE. Then, the mixture was stirred at room temperature for 1 h. After the reaction was completely finished, all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (60-90 °C)/EtOAc, 20:1) to afford the corresponding **3b** (137 mg, 64%) as a white solid.

## 5.2 Steric hindrance competition experiments



Under an air atmosphere, equal equivalent of diazo esters (**2b** and **21**) were added to a mixture of propargyl amine **1a** (284 mg, 1 mmol) and CuOTf (22 mg, 0.1 mmol) in DCE (10 mL). Then, the mixture was stirred at room temperature for 1 h. After the reaction was completely finished, all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (eluent: 60-90 °C)/EtOAc, 20:1) to afford the corresponding product of **3b** (91 mg) and **31** (53 mg).

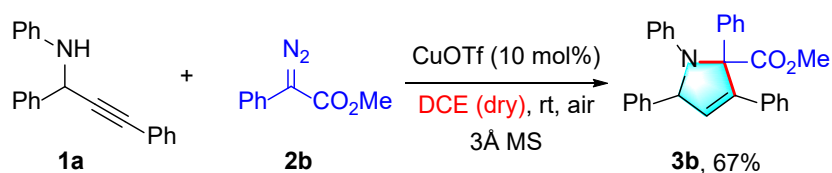
**Table S1.** Competition experiment between **2b** and **21**<sup>a</sup>

entry	yield of <b>3b</b>	yield of <b>31</b>	ratio
1	41%	23%	1.76:1

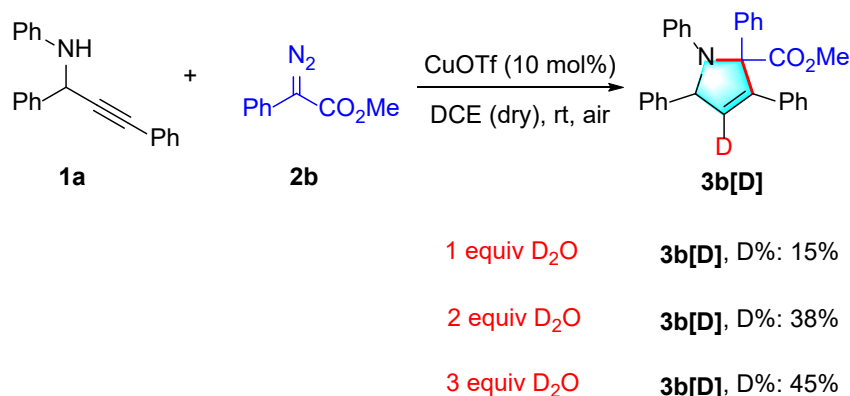
<sup>a</sup>Conditions: **1a** (1 mmol), **2b** (0.75 mmol), **21** (0.75 mmol), CuOTf (0.05 mmol), DCE (5 mL), 1 h, air (0.1 MPa), isolated yield.



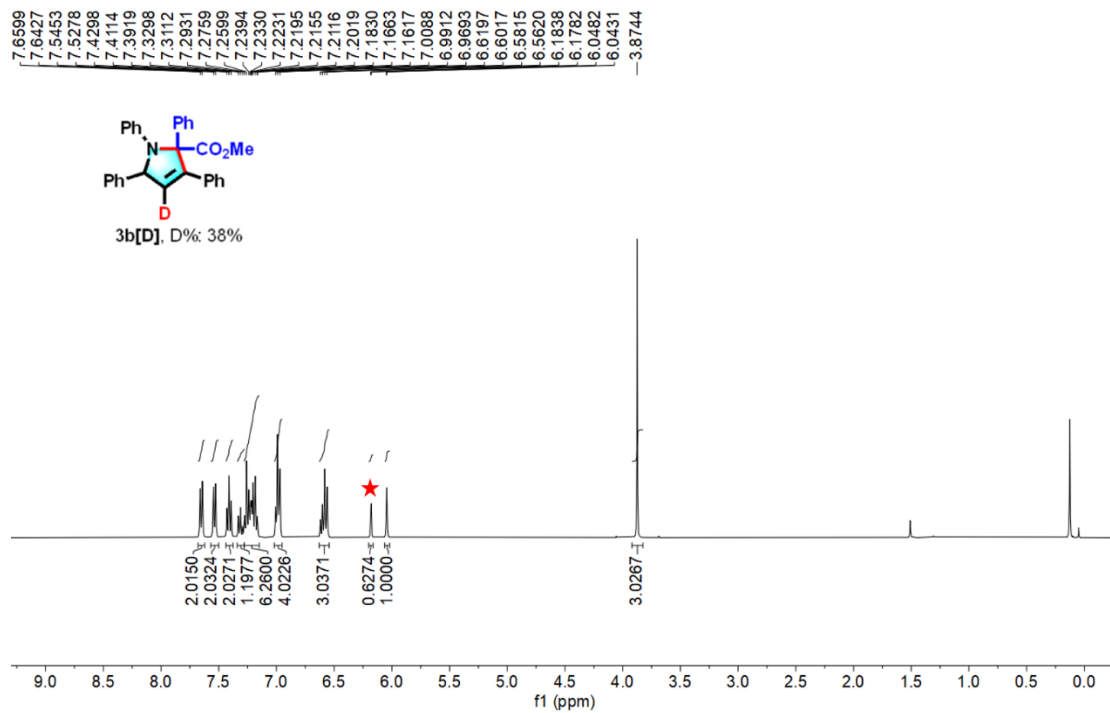
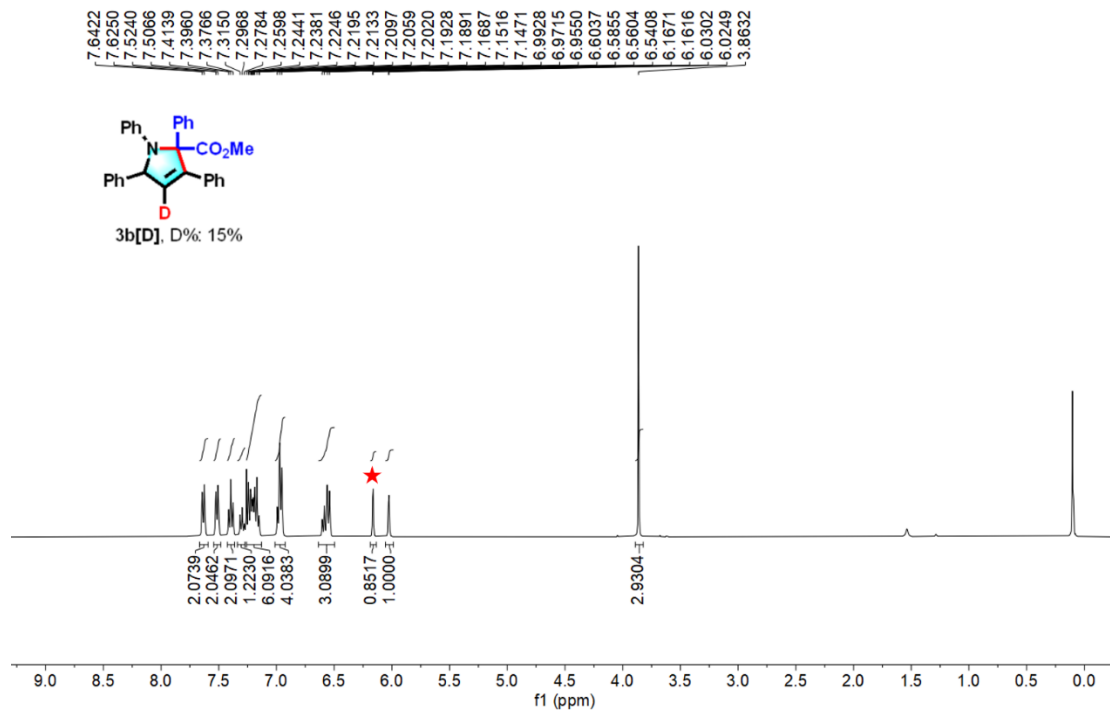
### 5.3 Deuterium isotope exchange experiments

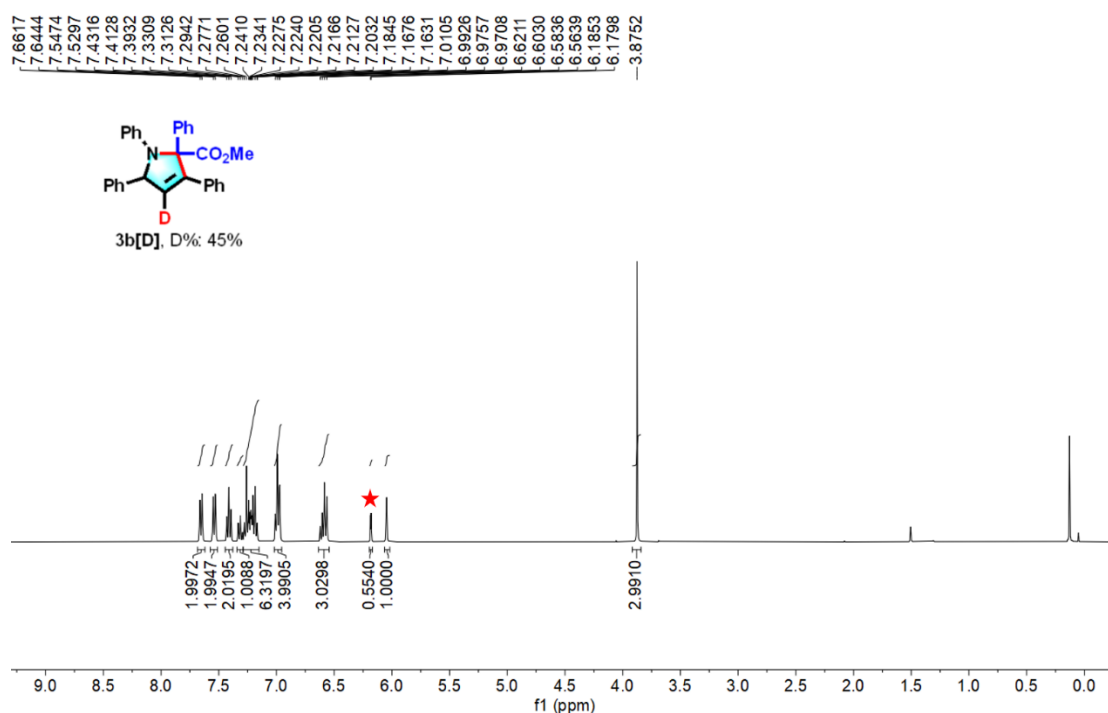


To avoid the effect of water in solvent, DCE was dried over CaH<sub>2</sub> and distilled. Under an air atmosphere, methyl 2-diazo-2-phenylacetate **2b** (132 mg, 0.75 mmol in 1 mL of DCE) was added slowly to a mixture of propargyl amine **1a** (142 mg, 0.5 mmol) and CuOTf (11 mg, 0.05 mmol) in 4 mL dry DCE. Then, the mixture was stirred at room temperature for 1 h. After the reaction was completely finished, all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (eluent: 60-90 °C)/EtOAc, 20:1) to afford the corresponding **3b** (145 mg, 67%) as a white solid.

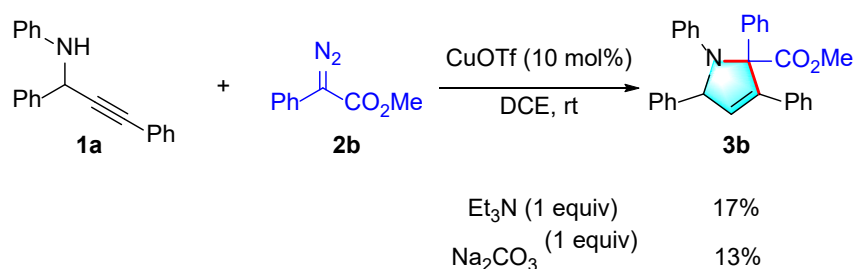


To avoid the effect of water in solvent, DCE was dried over CaH<sub>2</sub> and distilled. Under an air atmosphere, methyl 2-diazo-2-phenylacetate **2b** (132 mg, 0.75 mmol in 1 mL of DCE) was added slowly to a mixture of propargyl amine **1a** (142 mg, 0.5 mmol), CuOTf (11 mg, 0.05 mmol), and D<sub>2</sub>O (*x* equivalent, *x* = 1, 2 or 3) in 4 mL dry DCE. Then, the mixture was stirred at room temperature for 1 h. After the reaction was completely finished, all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (60-90 °C)/EtOAc, 20:1) to afford the corresponding **3b[D]** as a white solid and the <sup>1</sup>H NMR spectra were recorded.



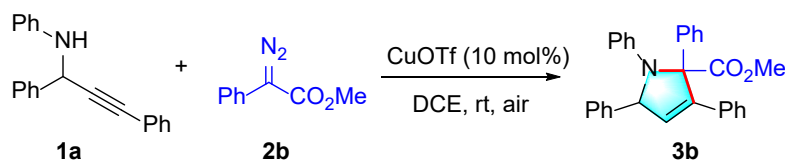


#### 5.4 With one equivalent base as additive



Under an air atmosphere, methyl 2-diazo-2-phenylacetate **2b** (132 mg, 0.75 mmol in 1 mL of DCE) was added slowly to a mixture of propargyl amine **1a** (142 mg, 0.5 mmol), CuOTf (11 mg, 0.05 mmol), and base (0.5 mmol) in 4 mL DCE. Then, the mixture was stirred at room temperature for 1 h. After the reaction was completely finished, all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (60-90 °C)/EtOAc, 20:1) to afford the corresponding **3b** as a white solid.

## 5.5 Online detection of pH experiments



Under an air atmosphere, methyl 2-diazo-2-phenylacetate **2b** (132 mg, 0.75 mmol in 1 mL of DCE) was added slowly to a mixture of propargyl amine **1a** (142 mg, 0.5 mmol),  $\text{CuOTf}$  (11 mg, 0.05 mmol) in 4 mL DCE. Then, the mixture was stirred at room temperature for 1 h. During this reaction, the pH of reaction solution was monitored, and the results were presented in Figure S1.

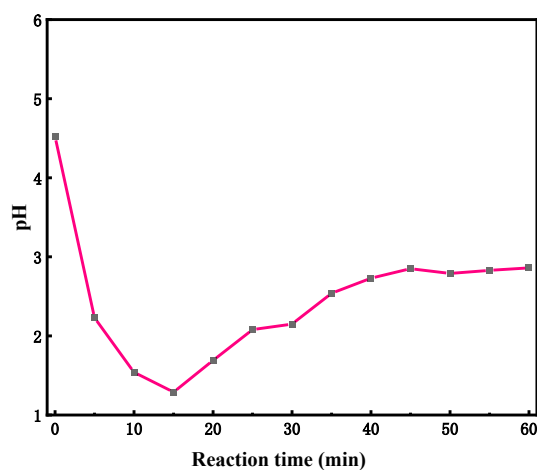
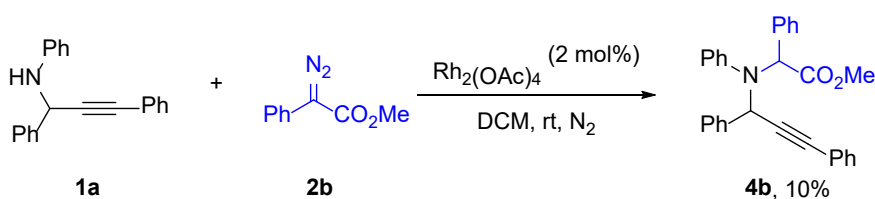


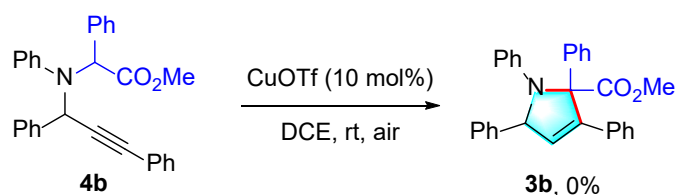
Figure S1. The detection of pH in reaction system

## 5.6 Intermediate trap experiments

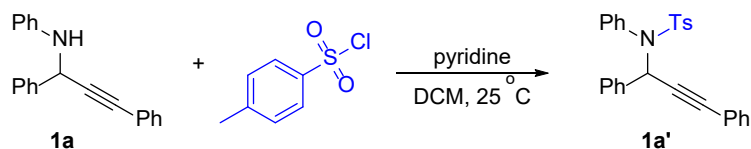


Under a  $\text{N}_2$  atmosphere, methyl 2-diazo-2-phenylacetate **2b** (264 mg, 1.5 mmol in 1 mL of DCM) was added slowly to a mixture of propargyl amine **1a** (284 mg, 1 mmol) and  $\text{Rh}_2(\text{OAc})_4$  (9 mg, 0.02 mmol) in 4 mL DCM. Then, the mixture was stirred at room temperature for 12 h. After **1a** was completely consumed by TLC monitoring on silica gel, the resultant mixture was cooled to ambient temperature and all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography

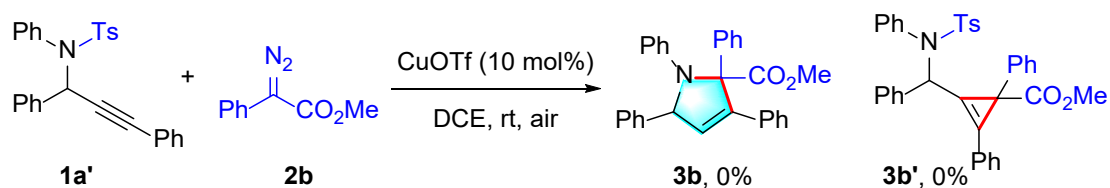
(eluent: petroleum ether (60-90 °C)/EtOAc, 20:1) to afford the coupled product **4b** (42 mg, 10%) as a white solid.



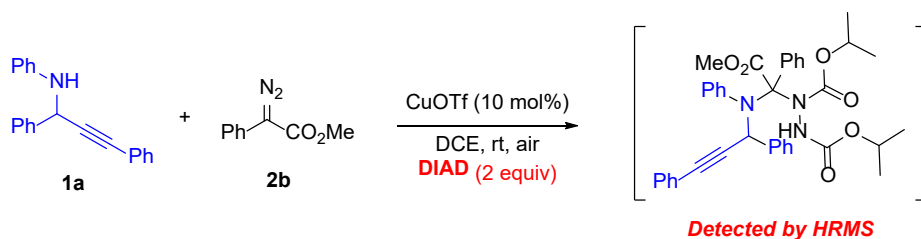
Under an air atmosphere, a mixture of **4b** (216 mg, 0.5 mmol), and CuOTf (11 mg, 0.05 mmol) in DCE (5 mL) was stirred at room temperature for 1 h. After monitoring on silica gel, no reaction occurred in this system.



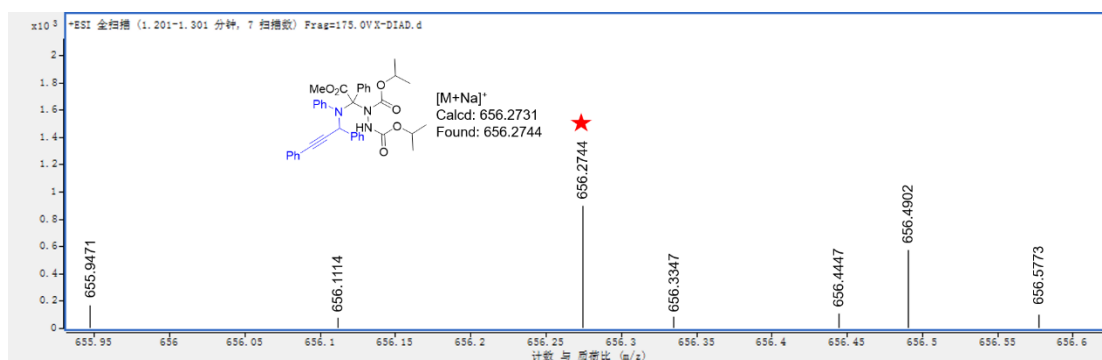
Under an air atmosphere, a mixture of **1a** (142 mg, 0.5 mmol), TsCl (115 mg, 0.6 mmol), and pyridine (158 mg, 2 mmol) in DCM (5 mL) was stirred at room temperature for 6 h. After monitoring on silica gel, all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (60-90 °C)/EtOAc, 10:1) to afford the desired product **1a'** (175 mg, 81%) as a white solid.



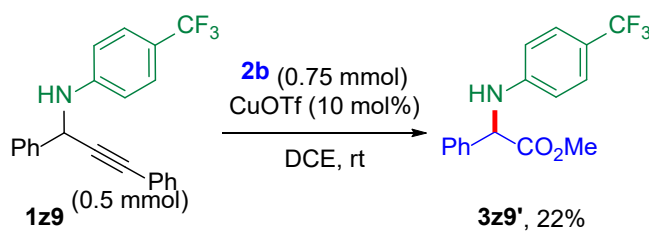
Under an air atmosphere, methyl 2-diazo-2-phenylacetate **2b** (132 mg, 0.75 mmol in 1 mL of DCE) was added slowly to a mixture of **1a'** (219 mg, 0.5 mmol) and CuOTf (11 mg, 0.05 mmol) in 4 mL DCE. Then, the mixture was stirred at room temperature for 1 h. After TLC monitoring on silica gel, no reaction occurred in this system.



Under the standard conditions, diisopropyl azodicarboxylate (DIAD) was used as the ylide trapping agent to perform the insertion reaction: methyl 2-diazo-2-phenylacetate **2b** (132 mg, 0.75 mmol in 1 mL of DCE) was added slowly to a mixture of propargyl amine **1a** (142 mg, 0.5 mmol), CuOTf (11 mg, 0.05 mol), and DIAD (203  $\mu\text{L}$ , 1 mmol) in 4 mL of DCE. Then, the reaction mixture was stirred at room temperature for 1 h. After TLC monitoring on silica gel, the reaction was completely suppressed and *N*-ylide intermediate was detected by HRMS (Figure S2).



**Figure S2.** The HRMS spectrum of *N*-ylide intermediate



Under an air atmosphere, methyl 2-diazo-2-phenylacetate **2b** (132 mg, 0.75 mmol in 1 mL of DCE) was added slowly to a mixture of propargyl amine **1z9** (142 mg, 0.5 mmol), CuOTf (11 mg, 0.05 mmol) in 4 mL DCE. Then, the mixture was stirred at room temperature for 1 h. After the reaction was completely finished, all the volatiles were evaporated under reduced pressure. The residue was purified by flash chromatography (eluent: petroleum ether (60-90 °C)/EtOAc, 10:1) to afford C–N

cleavage product **3z9'** as a white solid (34 mg, 22%).

## 6. DFT studies

### 6.1 Computational methodology

All computations were performed with the Gaussian16 program suite.<sup>[13]</sup> Geometries were optimized in the gas phase with the B3LYP<sup>[14]</sup> functional combining a def2-SVP<sup>[15]</sup> basis set. Harmonic frequency calculations were performed for each stationary point to ensure that it is either an energy minimum (no imaginary frequency) or a transition state (only one imaginary frequency) and to present the thermodynamic energy corrections. For each transition state, intrinsic reaction coordinate (IRC) analysis<sup>[16]</sup> was performed to ensure that it connects the correct reactant and product. To take the solvent effect into account, single-point energy calculations in the solution phase with an SMD solvation model (solvent=DCE)<sup>[17]</sup> were performed on the basis of the gas phase-optimized structures by using the the B3LYP functional combining a def2-TZVP basis set<sup>[15]</sup>. In the geometry optimization and single-point calculations, dispersion corrections [DFT-D3(BJ)]<sup>[18]</sup> were added to better describe long-range weak interactions. Wavefunction analysis was conducted with the Multiwfn (Multifunctional Wavefunction Analyzer)<sup>[19]</sup> including orbital composition analysis with Mulliken partition. In this way, the coefficients on each carbon atom were not simply squared and summed up. Here, the Mulliken partition for calculating orbital components corresponded to the method used by Mulliken population method. In Mulliken population method, the population of a basis function of an orbit was the contribution value of the basis function multiplied by the orbital occupancy. Visualization of the frontier molecular orbitals orbitals was carried out by GaussView.<sup>[20]</sup> The single-point energies corrected by the thermal correction to Gibbs free energies (TCG, obtained from frequency calculations) were used as the Gibbs free energies at 298.15 K and 1 atm in kcal mol<sup>-1</sup>. The 3-D images of the calculated structures were prepared using CYLview 1.0b<sup>[21]</sup>.

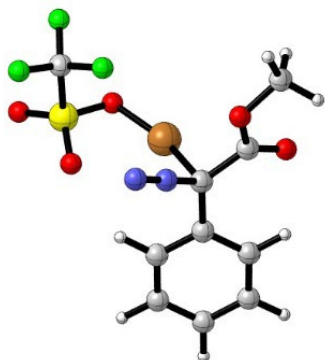
## 6.2 Computed Energies for all the structures

Zero-point correction (ZPE), thermal correction to enthalpy (TCH), thermal correction to Gibbs free energy (TCG), single-point energy (SPE) and Gibbs free energies ( $\Delta G$ ) (in Hartree) of the structures, and the imaginary frequency (in  $\text{cm}^{-1}$ ) of all the transition states are given.

Structure	ZPE	TCH	TCG	SPE	$\Delta G$	IF
<b>CuOTf+2b</b>	0.187846	0.211435	0.131170	-3210.394058	-3210.262888	None
<b>TS1</b>	0.185592	0.209218	0.129674	-3210.380243	-3210.250569	-429.13
<b>N<sub>2</sub></b>	0.005674	0.008978	-0.012767	-109.568246	-109.581013	None
<b>A</b>	0.178263	0.199833	0.123459	-3100.843480	-3100.720021	None
<b>1a</b>	0.317876	0.337113	0.264287	-865.591967	-865.327680	None
<b>B</b>	0.501707	0.541622	0.424186	-3966.478432	-3966.054246	None
<b>TS2</b>	0.499445	0.539205	0.423208	-3966.469612	-3966.046404	-284.82
<b>C</b>	0.498004	0.538784	0.420321	-3966.483786	-3966.063465	None
<b>TS3</b>	0.496968	0.537161	0.419819	-3966.478509	-3966.058690	-54.48
<b>D</b>	0.499677	0.539820	0.422230	-3966.517322	-3966.095092	None
<b>TS4</b>	0.501731	0.540271	0.427411	-3966.508148	-3966.080737	-58.51
<b>E</b>	0.504221	0.542737	0.430604	-3966.514999	-3966.084395	None
<b>C'</b>	0.498106	0.538801	0.419184	-3966.487264	-3966.068080	None
<b>TS5</b>	0.498326	0.538126	0.421485	-3966.486581	-3966.065096	-66.83
<b>F</b>	0.501565	0.541066	0.424665	-3966.524756	-3966.100091	None
<b>TS6</b>	0.500823	0.539909	0.423816	-3966.490855	-3966.067039	-183.53
<b>G</b>	0.503570	0.542204	0.428754	-3966.513280	-3966.084526	None
<b>H</b>	0.461163	0.491080	0.398902	-3004.093888	-3003.694986	None
<b>CF<sub>3</sub>SO<sub>3</sub>H</b>	0.038852	0.047584	0.005741	-962.368280	-962.362539	None
<b>TS7</b>	0.497824	0.536271	0.422433	-3966.477706	-3966.055273	-78.30
<b>TS8</b>	0.496977	0.535551	0.422163	-3966.441228	-3966.019065	-1347.60
<b>I</b>	0.500758	0.539529	0.425495	-3966.486732	-3966.061237	None
<b>TS9</b>	0.497890	0.536588	0.421931	-3966.480070	-3966.058139	-657.69
<b>CuOTf+3b</b>	0.502066	0.541016	0.427053	-3966.543353	-3966.116300	None



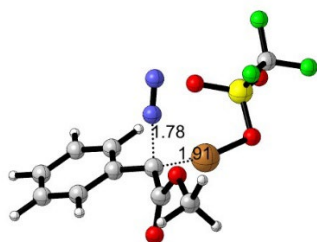
### 6.3 CYLview Structures and cartesian coordinates of the optimized geometries



#### CuOTf+2b

Cu	0.03659000	0.00762400	-0.88742200
O	-1.61580000	-0.72427800	-1.56382000
S	-2.31292400	-1.27630100	-0.31435400
O	-3.28148300	-2.32441000	-0.58243200
O	-1.32659000	-1.45363700	0.78159500
C	-3.27651400	0.22497500	0.24209800
F	-4.12767500	0.62578900	-0.69364400
F	-3.94491300	-0.03985000	1.35833700
F	-2.41329200	1.22879000	0.49180600
C	1.47365000	0.66321800	0.36915700
C	1.76366500	2.01862000	-0.19777200
C	2.41019200	-0.51486500	0.27245400
C	3.71075900	-0.37130500	-0.23670600
C	1.96116400	-1.78272000	0.69105800
C	4.54859700	-1.48554000	-0.31616200
H	4.05453200	0.60084800	-0.58452600
C	2.81404600	-2.88346900	0.61654400
H	0.93620300	-1.91424500	1.04699800
C	4.10991300	-2.74055900	0.11282200
H	5.55772100	-1.36549500	-0.71698400
H	2.45375200	-3.86150800	0.94266500
H	4.77278300	-3.60617200	0.04752700
O	1.03203800	2.96213100	0.41478700

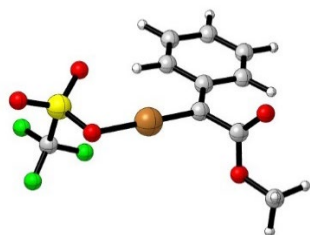
O	2.53304500	2.22867100	-1.10240500
C	1.14574300	4.29253800	-0.10304300
H	0.49518000	4.91431500	0.52223500
H	2.18669600	4.64132900	-0.04644900
H	0.81550100	4.32476500	-1.15166900
N	0.75799500	0.71725500	1.53130600
N	0.14904300	0.72562400	2.47042300



### TS1

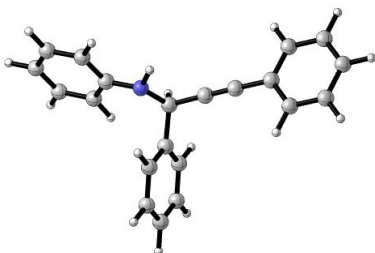
Cu	-0.12175600	0.22684300	-0.99012600
O	-1.89587800	-0.21499700	-1.57882900
S	-2.52170700	-1.04470800	-0.45138400
O	-3.55537000	-1.96532000	-0.89186200
O	-1.46815800	-1.51903900	0.47987500
C	-3.37869800	0.29425800	0.52911000
F	-4.29739600	0.91119600	-0.20341600
F	-3.95402900	-0.21980100	1.61055600
F	-2.46744700	1.20286200	0.92388400
C	1.54150600	0.48024600	-0.07942400
C	2.12047600	1.82663500	-0.34142500
C	2.41573200	-0.69841700	0.07516800
C	3.81686900	-0.58001100	0.17715800
C	1.82639900	-1.98053800	0.12259800
C	4.60802000	-1.72020000	0.29804600
H	4.28475100	0.40294200	0.12297400
C	2.62294800	-3.11320400	0.27022400
H	0.73812600	-2.07567000	0.06762100
C	4.01398300	-2.98601100	0.35069700
H	5.69424300	-1.62226400	0.35600300

H	2.15685100	-4.09971900	0.31326300
H	4.63858800	-3.87670100	0.45262800
O	1.58221500	2.80794900	0.39583500
O	2.93682300	1.99840000	-1.21592200
C	1.98684800	4.14037100	0.06350200
H	1.47107800	4.79736600	0.77313100
H	3.07689000	4.24967000	0.15759000
H	1.69417500	4.38401900	-0.96836400
N	0.79290300	0.66796100	1.52837200
N	0.11450000	0.48835300	2.38234700
<b>N<sub>2</sub></b>			
N	0.00000000	0.00000000	0.55019600
N	0.00000000	0.00000000	-0.55019600



<b>A</b>			
Cu	0.03741200	-0.96030200	-0.57353500
O	1.88437400	-1.36816500	-0.73391000
S	2.73390700	-0.08704200	-0.77159300
O	4.03823300	-0.27530100	-1.38268100
O	1.90951100	1.07730100	-1.15724700
C	3.03073300	0.16829700	1.05506000
F	3.68078800	-0.86058800	1.58545400
F	3.73254900	1.27926100	1.25698600
F	1.84684400	0.29436400	1.67916500
C	-1.70712000	-0.40499800	-0.26597600
C	-2.75280000	-1.44522400	-0.17001300
C	-2.08367300	0.95999500	-0.12898600
C	-3.42978000	1.36060000	0.12585200

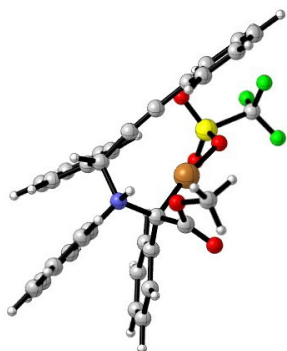
C	-1.07558800	1.96514000	-0.22565900
C	-3.74463300	2.69922400	0.28625200
H	-4.21431300	0.60356000	0.17256000
C	-1.40261300	3.30392700	-0.05267800
H	-0.04230400	1.67228200	-0.43539400
C	-2.73046500	3.66921000	0.20138300
H	-4.77566900	3.00377300	0.47651900
H	-0.62526700	4.06699700	-0.12270000
H	-2.98521000	4.72425000	0.33122600
O	-2.68066000	-2.14897400	0.96093300
O	-3.53431800	-1.64982300	-1.07164400
C	-3.60139400	-3.23978300	1.09532100
H	-3.39897000	-3.68531000	2.07578300
H	-4.64012100	-2.88197300	1.04221100
H	-3.44035700	-3.97810000	0.29640100



**1a**

C	0.52370100	-0.06533600	-0.47783500
H	0.79865700	-0.27371400	-1.53308500
C	-0.92469400	-0.26380900	-0.35519800
C	-2.12549100	-0.40874500	-0.24202900
C	-3.54091700	-0.56794600	-0.10551600
C	-4.27421000	0.28072400	0.74874300
C	-4.22430000	-1.57193800	-0.82109300
C	-5.65331800	0.12590700	0.88074500
H	-3.74704100	1.05956900	1.30276200
C	-5.60363700	-1.72035400	-0.68324600
H	-3.65941700	-2.23012200	-1.48385300

C	-6.32206800	-0.87353800	0.16673200
H	-6.21117000	0.78988500	1.54530500
H	-6.12251500	-2.50203900	-1.24310900
H	-7.40296100	-0.99229000	0.27247200
C	0.87194300	1.40335100	-0.20496500
C	1.24287100	1.82154600	1.07586100
C	0.78739400	2.34201100	-1.23915400
C	1.52596500	3.16727400	1.32077000
H	1.32064300	1.07747100	1.87059100
C	1.06846700	3.68819400	-0.99548300
H	0.49940300	2.01600500	-2.24274900
C	1.43849900	4.10415400	0.28700900
H	1.82094900	3.48570700	2.32370400
H	1.00289600	4.41390300	-1.80981100
H	1.66365400	5.15604900	0.47856600
N	1.22008200	-0.99155700	0.39981200
H	0.63169000	-1.68635600	0.84053700
C	2.54314500	-1.35453100	0.19552100
C	3.40274400	-0.61559400	-0.64181600
C	3.06220900	-2.48669400	0.85905600
C	4.73344900	-1.00845700	-0.80403500
H	3.04240600	0.27836900	-1.14972500
C	4.39089300	-2.86443200	0.68862000
H	2.40634000	-3.06890400	1.51278200
C	5.24139300	-2.12994500	-0.14617400
H	5.38205700	-0.41839500	-1.45677400
H	4.76630000	-3.74698900	1.21308300
H	6.28331200	-2.42829400	-0.27845400

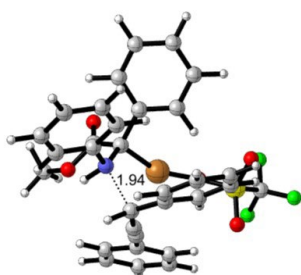


**B**

C	1.41503900	0.49653900	-0.85947200
C	1.29436400	1.63084500	-1.80879400
C	2.10252500	-0.72445500	-1.41270900
C	3.21817300	-0.60038600	-2.26000000
C	1.67255400	-2.01604300	-1.06841200
C	3.89984500	-1.72618200	-2.72016300
H	3.55689900	0.39235500	-2.55968200
C	2.36257600	-3.14585000	-1.51341700
H	0.77954500	-2.14619800	-0.45768500
C	3.48317900	-3.00456600	-2.33549900
H	4.76353500	-1.60560800	-3.37854900
H	2.00700600	-4.13808800	-1.22712400
H	4.01992000	-3.88760200	-2.69097400
O	1.27537700	2.84911900	-1.14891800
O	1.17392000	1.56450000	-3.00814300
C	0.84987600	3.98142100	-1.90357400
H	1.35624900	4.00823400	-2.87787900
H	-0.23870900	3.93841400	-2.06559600
H	1.10358900	4.86757600	-1.30824000
C	1.29659200	0.72808000	1.81692900
H	1.93365700	1.25989200	2.54064600
C	-0.00236400	1.37372600	1.71600800
C	-1.06829300	1.92884900	1.52594100
C	-2.32351500	2.54710300	1.24223500
C	-3.50034000	1.77197500	1.20811700

C	-2.38259100	3.92421200	0.94504900
C	-4.71131700	2.37476200	0.87280100
H	-3.45162200	0.70360800	1.41849300
C	-3.60107900	4.51458300	0.61684800
H	-1.46604400	4.51718700	0.97034200
C	-4.76647100	3.74049300	0.57844600
H	-5.61522400	1.76382000	0.82840000
H	-3.64364800	5.58154900	0.38603100
H	-5.71956500	4.20444000	0.31335900
C	1.23667900	-0.73492700	2.18673800
C	0.08040000	-1.48041300	1.93595200
C	2.33076200	-1.35931100	2.80494200
C	0.03502800	-2.84690300	2.21345100
H	-0.81392700	-0.99113500	1.55841400
C	2.28891700	-2.72508200	3.08802400
H	3.21628200	-0.77777500	3.06755300
C	1.14853600	-3.47470400	2.77473800
H	-0.87591000	-3.39766600	1.97479000
H	3.14717600	-3.20589000	3.56309300
H	1.12286700	-4.54498300	2.99274700
C	3.49122000	1.00747100	0.53918900
C	4.20208200	-0.19310100	0.61007100
C	4.16098300	2.23434100	0.52159500
C	5.59565000	-0.15156700	0.68210000
H	3.68316500	-1.14661000	0.59566000
C	5.55499700	2.26472000	0.59006700
H	3.59186500	3.16284600	0.43853500
C	6.27414000	1.06976100	0.67330500
H	6.15256500	-1.08927600	0.73258900
H	6.07625300	3.22403500	0.57480600
H	7.36486500	1.09047900	0.72480200
N	2.02995600	1.04124800	0.45199000
H	1.79293000	2.03970300	0.33872300
Cu	-0.52105400	0.10126700	-0.69850100

O	-2.08552600	-2.89511600	-0.48448900
S	-2.83868600	-1.69439500	-0.10885600
O	-3.11018500	-1.49148200	1.32644900
O	-2.35665500	-0.42335600	-0.79857100
C	-4.52347200	-1.85322000	-0.88819100
F	-4.42338700	-1.96525000	-2.20868700
F	-5.13594200	-2.93262200	-0.40699700
F	-5.26149000	-0.77777100	-0.60025700



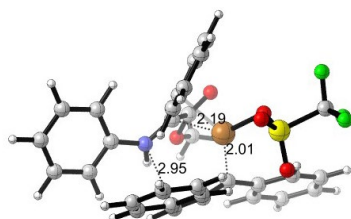
## TS2

C	-1.32809100	0.80729700	0.80799500
C	-1.06987600	2.07646000	1.53385500
C	-1.79198700	-0.33728900	1.67576300
C	-2.79229500	-0.12975000	2.64111900
C	-1.27970300	-1.63561900	1.52017000
C	-3.28181200	-1.18704900	3.40696100
H	-3.19338200	0.87433500	2.78916800
C	-1.77201400	-2.69895700	2.28081100
H	-0.47660900	-1.83219700	0.80893300
C	-2.77977700	-2.47947200	3.22220500
H	-4.06093500	-1.00266200	4.15061800
H	-1.34886000	-3.69587300	2.13985000
H	-3.16331100	-3.30862800	3.82183400
O	-1.20722000	3.17746300	0.71423800
O	-0.75101200	2.19374400	2.69444500
C	-0.84310800	4.43004200	1.28821700
H	-1.42311000	4.62592600	2.20147900
H	0.22681000	4.43902800	1.54538100



H	-1.05634100	5.19122300	0.52699900
C	-1.33752100	0.59107400	-2.12528100
H	-2.09299100	1.14956100	-2.68944200
C	-0.07460900	1.20964600	-2.00229300
C	0.98016600	1.70870600	-1.62528500
C	2.20639200	2.35901800	-1.28905300
C	3.42187600	1.64423800	-1.28790900
C	2.19177100	3.72101500	-0.92011400
C	4.59774500	2.29013900	-0.91404400
H	3.42328600	0.58704500	-1.55310900
C	3.37564100	4.35415500	-0.55102900
H	1.24509500	4.26325500	-0.92339700
C	4.57906000	3.63886700	-0.54455800
H	5.53286100	1.72683600	-0.89645000
H	3.36238300	5.40783300	-0.26322600
H	5.50518100	4.13582100	-0.24602100
C	-1.40492100	-0.86738000	-2.29048900
C	-0.32243700	-1.67689800	-1.90693900
C	-2.58011300	-1.47554000	-2.77404900
C	-0.42540800	-3.06571300	-1.94358900
H	0.62302100	-1.22259900	-1.61908000
C	-2.67575600	-2.86441400	-2.82794900
H	-3.41752400	-0.85511000	-3.09868600
C	-1.60646100	-3.66074500	-2.39666700
H	0.42508100	-3.66184200	-1.60857400
H	-3.58950300	-3.33092800	-3.20304200
H	-1.69143500	-4.74955700	-2.43049500
C	-3.52066000	0.76353500	-0.45434600
C	-4.01723000	-0.53302600	-0.27101200
C	-4.39794700	1.81781500	-0.74304500
C	-5.39187800	-0.75702200	-0.36083700
H	-3.34309900	-1.35738400	-0.06149600
C	-5.76998400	1.58268000	-0.83552200
H	-4.00141300	2.82807800	-0.87516500

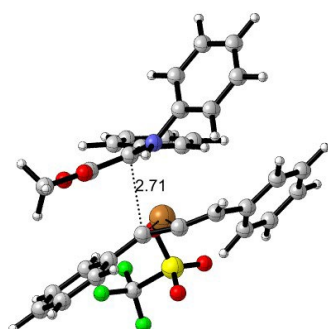
C	-6.27072400	0.29195400	-0.64177900
H	-5.77459100	-1.76854700	-0.21028000
H	-6.44750000	2.41139400	-1.05208100
H	-7.34467300	0.10529000	-0.70948600
N	-2.11712800	1.06000200	-0.41081700
H	-2.00193200	2.06491900	-0.57000700
Cu	0.61352600	0.37249300	0.49098900
O	1.93345800	-2.89499200	0.47705000
S	2.72190400	-1.73594000	0.04234100
O	2.91824700	-1.56626000	-1.40974700
O	2.34646500	-0.43740300	0.74087200
C	4.43870900	-1.97567500	0.72493600
F	4.41128100	-2.06739500	2.05010500
F	4.96537900	-3.09043700	0.22377100
F	5.21210300	-0.94277400	0.37868100



<b>C</b>			
C	-1.42929400	1.21579700	1.13893200
C	-0.78295300	2.49550400	1.54438800
C	-1.11968300	-0.06413300	1.80333700
C	-0.44258700	-0.14763300	3.04559200
C	-1.37716100	-1.27300800	1.09045400
C	-0.01094700	-1.38264500	3.52295700
H	-0.22851600	0.76379500	3.59847400
C	-0.92436100	-2.49119900	1.57600200
H	-1.88954900	-1.23607200	0.13010200
C	-0.23158000	-2.55112900	2.79020100
H	0.53003200	-1.42670100	4.47045900

H	-1.07682500	-3.39141600	0.98032000
H	0.15436300	-3.50673000	3.14936100
O	-1.29796700	3.54190200	0.86282300
O	0.10221600	2.61879800	2.36554600
C	-0.69351700	4.81282000	1.12236200
H	-0.83449300	5.09659900	2.17525900
H	0.38221800	4.77889100	0.90154900
H	-1.19948000	5.52732900	0.46234200
C	-1.55977900	0.43029700	-2.36074300
H	-2.45341500	1.01128200	-2.60428600
C	-0.46144100	1.07874800	-1.92448200
C	0.52609600	1.56973800	-1.29221500
C	1.69366200	2.42465100	-1.34676500
C	2.99189500	1.91194700	-1.14470000
C	1.52437500	3.80762900	-1.56811000
C	4.08826600	2.77102400	-1.16831700
H	3.12709300	0.84305100	-0.98896700
C	2.62915300	4.65716500	-1.58631700
H	0.51815500	4.19884400	-1.72975900
C	3.91440400	4.14282500	-1.38232200
H	5.08932400	2.36112900	-1.01654800
H	2.48850200	5.72617400	-1.76443900
H	4.77907800	4.81045800	-1.39353600
C	-1.65024200	-1.01820400	-2.47542700
C	-0.51923500	-1.84025000	-2.27697600
C	-2.90859000	-1.62921700	-2.65884300
C	-0.65115200	-3.22244300	-2.21573100
H	0.46823000	-1.39389700	-2.15223800
C	-3.03415200	-3.01767800	-2.60715100
H	-3.79281000	-1.00590100	-2.80860400
C	-1.91033800	-3.81855000	-2.37679400
H	0.23603900	-3.82560100	-2.01426600
H	-4.01709200	-3.47702200	-2.73682900
H	-2.01368800	-4.90498400	-2.32424400

C	-3.76950700	0.70995000	0.35571100
C	-4.20466100	-0.05573000	1.45071500
C	-4.65309900	0.92490100	-0.71691600
C	-5.48112500	-0.61818600	1.44285500
H	-3.55780500	-0.20605300	2.31203400
C	-5.92983100	0.36769300	-0.70899900
H	-4.33269600	1.53908000	-1.56098700
C	-6.34942500	-0.42075800	0.36603900
H	-5.80124900	-1.21340300	2.30114500
H	-6.59905300	0.54949700	-1.55308300
H	-7.34558800	-0.86737800	0.36939700
N	-2.50448600	1.32325400	0.29188700
H	-2.47586600	2.16524000	-0.27410800
Cu	0.45162800	0.41516700	0.35010500
O	1.78125100	-3.13890600	0.12356100
S	2.46318300	-1.86145300	-0.10408100
O	2.66395600	-1.42680600	-1.49665200
O	1.97150400	-0.73177900	0.79283800
C	4.18190900	-2.07685600	0.58366200
F	4.13179600	-2.39078500	1.87666200
F	4.80827600	-3.05102500	-0.07202200
F	4.87882700	-0.94704300	0.44215700

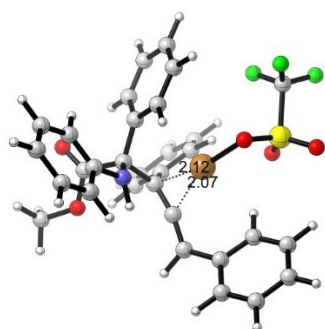


### TS3

C	-1.55503600	1.42377100	0.88794700
C	-0.84439700	2.71032700	1.04908400
C	-1.18246600	0.21921500	1.64688600

C	-0.40251600	0.27472500	2.82557800
C	-1.57186800	-1.05965900	1.15914700
C	-0.02040000	-0.89916600	3.47259400
H	-0.07929400	1.24150100	3.20293000
C	-1.16565000	-2.22254500	1.80844000
H	-2.18195400	-1.14371000	0.26317600
C	-0.38828100	-2.14863800	2.96852700
H	0.59482600	-0.83385800	4.37230200
H	-1.44507600	-3.18929900	1.38586400
H	-0.05708500	-3.06210800	3.46596000
O	-1.42505000	3.68982900	0.31059100
O	0.11548300	2.91171100	1.76311500
C	-0.85202200	4.99275600	0.44489100
H	-1.00195800	5.37087800	1.46749300
H	0.22287000	4.97065400	0.22480400
H	-1.37718700	5.62981000	-0.27677600
C	-1.55858300	-0.11078000	-2.33475200
H	-2.41003100	0.37028800	-2.82628900
C	-0.57802400	0.66419700	-1.82283500
C	0.21143500	1.42398500	-1.16598300
C	1.24302200	2.41788600	-1.16963600
C	2.36069500	2.30690700	-0.31538000
C	1.11988300	3.55619300	-1.99774900
C	3.33745500	3.29907300	-0.30935200
H	2.46741600	1.42763600	0.32010900
C	2.09625300	4.54737200	-1.97506400
H	0.25210700	3.64391400	-2.65430500
C	3.20782800	4.42325500	-1.13060700
H	4.20605600	3.18986200	0.34324500
H	1.99746900	5.42083000	-2.62420300
H	3.97431000	5.20159800	-1.11884900
C	-1.54650000	-1.56712400	-2.21971700
C	-0.33959300	-2.26242000	-1.97537500
C	-2.75240100	-2.29433500	-2.22487700

C	-0.34621400	-3.61925300	-1.66851100
H	0.61909000	-1.74110500	-2.05065000
C	-2.75375600	-3.66011900	-1.93087100
H	-3.69456700	-1.77501500	-2.41518400
C	-1.55809700	-4.32372100	-1.63542200
H	0.60295700	-4.11178300	-1.44428500
H	-3.69931100	-4.20788800	-1.92017000
H	-1.56737500	-5.38879500	-1.39283900
C	-3.89997300	0.74468800	0.30638700
C	-4.30894000	0.25881500	1.55836500
C	-4.74860800	0.59680600	-0.80133200
C	-5.53246900	-0.39955400	1.67968400
H	-3.67557400	0.40049600	2.43287200
C	-5.97741200	-0.04707500	-0.66593700
H	-4.43260600	0.98203100	-1.77264700
C	-6.37102700	-0.56122800	0.57322500
H	-5.83736300	-0.77913200	2.65750500
H	-6.62690600	-0.15447800	-1.53762500
H	-7.32813100	-1.07612400	0.67758000
N	-2.67905800	1.43424500	0.12669200
H	-2.72698300	2.23202000	-0.50210600
Cu	0.51329800	-0.29775800	-0.11863400
O	2.87901700	-3.35173800	-0.12101800
S	2.89632100	-1.88946800	-0.14230100
O	2.85714400	-1.20304000	-1.44745500
O	1.91825400	-1.25215600	0.84552300
C	4.52139100	-1.38684500	0.62098900
F	4.64166800	-1.89698100	1.84447700
F	5.53095100	-1.82013400	-0.12910400
F	4.59513400	-0.05325800	0.70644200



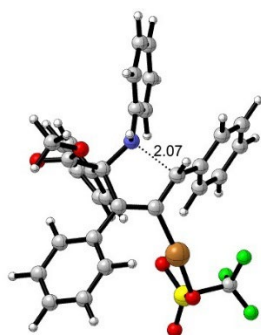
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C	-1.94930200	0.30239700	-0.19075500
C	-3.29345800	0.63060600	-0.89727800
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C	-1.45972400	2.78900100	0.22827500
C	-0.64593400	1.14707600	1.80547000
C	-0.78866100	3.78736400	0.93739400
H	-2.03100100	3.05082200	-0.65873500
C	0.03925500	2.14606600	2.49986300
H	-0.60719300	0.11857700	2.16547000
C	-0.02967200	3.47044800	2.06667400
H	-0.84825700	4.82122000	0.58992700
H	0.64116200	1.87712300	3.36964800
H	0.51385800	4.25218800	2.60156800
O	-3.67185400	-0.42189800	-1.64156100
O	-3.94475100	1.63403100	-0.78350200
C	-4.95147400	-0.31785500	-2.27172400
H	-5.73874700	-0.18210300	-1.51631500
H	-4.97316400	0.53847900	-2.96214100
H	-5.09949800	-1.25680700	-2.81755300
C	-0.16780500	-2.44987200	-1.93610700
H	-0.91449300	-2.88568600	-2.61421700
C	-0.40001400	-1.21720600	-1.51105500
C	-0.88214000	0.02150700	-1.29458500
C	-0.53433100	1.13858500	-2.23618500
C	0.64252500	1.88402600	-2.07918600
C	-1.41423000	1.44805600	-3.28404600

C	0.92501500	2.93609700	-2.95159100
H	1.35231000	1.64698400	-1.28407500
C	-1.13102000	2.50664000	-4.14918100
H	-2.31381800	0.84904400	-3.42966900
C	0.03701600	3.25569800	-3.98169900
H	1.84725900	3.50572800	-2.81964400
H	-1.82295500	2.74167600	-4.96120000
H	0.25850800	4.08296700	-4.65993600
C	0.97587300	-3.29173800	-1.54478100
C	2.21193100	-2.71442700	-1.20310400
C	0.83037500	-4.68704300	-1.46775500
C	3.25771300	-3.50312300	-0.72678500
H	2.37450000	-1.64392700	-1.34258400
C	1.88423400	-5.47866100	-1.00798300
H	-0.11993900	-5.14879300	-1.74873500
C	3.09281200	-4.88821000	-0.62328500
H	4.19160100	-3.02168700	-0.42947200
H	1.75889300	-6.56195000	-0.94102600
H	3.91048000	-5.50961100	-0.25092800
C	-3.10500500	-1.07175100	1.55956200
C	-3.81657700	0.00121600	2.12344600
C	-3.37810700	-2.37804100	2.00989900
C	-4.77260000	-0.24031800	3.11430400
H	-3.63205300	1.02300900	1.79785400
C	-4.33397300	-2.60452600	2.99614700
H	-2.82123000	-3.21620600	1.58151400
C	-5.04036400	-1.53548200	3.55893600
H	-5.31485900	0.60743100	3.54015100
H	-4.52732000	-3.62702100	3.32976500
H	-5.78890200	-1.71275200	4.33377400
N	-2.10751000	-0.91069900	0.58659200
H	-1.97726000	-1.74435500	0.02208500
Cu	0.73361300	-0.39716600	0.02057100
O	4.60908300	-0.82317800	1.07459200



S	3.49266600	0.04215700	0.71190400
O	3.31342900	0.41355900	-0.70980400
O	2.15664400	-0.37741900	1.32813900
C	3.79517400	1.66881700	1.57883500
F	3.65861600	1.53483900	2.89613900
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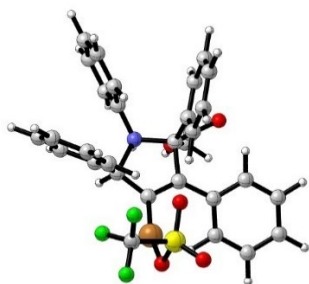


#### TS4

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C	-3.18357375	2.02458601	-0.18871701
C	-1.91870375	0.51452901	1.43277499
C	-3.02909875	0.31488501	2.26714199
C	-0.63704375	0.24632701	1.93135199
C	-2.85969375	-0.16118699	3.56701999
H	-4.03428975	0.52164001	1.90087799
C	-0.46803375	-0.23429399	3.23153399
H	0.25015725	0.41252901	1.32371599
C	-1.57858275	-0.44439199	4.05160999
H	-3.73422675	-0.31591499	4.20309899
H	0.54446025	-0.43521799	3.58784199
H	-1.44842575	-0.81944499	5.06970299
O	-3.53900675	2.13625301	-1.48641701
O	-3.63195975	2.72371701	0.67769199
C	-4.43736075	3.20313801	-1.80783101
H	-5.38742975	3.08418501	-1.26715301
H	-3.99027075	4.16876301	-1.53174001

H	-4.59867775	3.14967801	-2.89072701
C	-0.69901175	-0.65251899	-1.80146801
H	-1.16423475	-0.66310699	-2.79719301
C	-0.10919775	0.57662001	-1.40329401
C	-0.78203575	1.46457501	-0.64215401
C	-0.28391275	2.81388101	-0.29290401
C	-0.60280375	3.46308601	0.91423799
C	0.57185925	3.48107301	-1.19553101
C	-0.06354975	4.71616601	1.21436899
H	-1.26285875	2.98771401	1.63673199
C	1.11511625	4.72617601	-0.89061501
H	0.79896825	3.00718301	-2.15328301
C	0.80131525	5.35055201	0.32126199
H	-0.31697275	5.19278701	2.16412999
H	1.78257425	5.21464101	-1.60436301
H	1.22724925	6.32665501	0.56454999
C	-0.30243675	-1.98435699	-1.33645801
C	0.61267525	-2.16326699	-0.28195301
C	-0.91810775	-3.11386299	-1.90834501
C	0.89734225	-3.44238399	0.18697999
H	1.12779225	-1.30875999	0.15615099
C	-0.63895975	-4.39258199	-1.42998301
H	-1.63496575	-2.98032999	-2.72240301
C	0.26870025	-4.55791499	-0.37922501
H	1.62755425	-3.56448099	0.98945699
H	-1.12867475	-5.26096599	-1.87568401
H	0.49591225	-5.56007499	-0.00764701
C	-3.28227975	-1.32687399	-0.44027901
C	-2.80641875	-2.21693399	0.53395899
C	-4.51540575	-1.57296599	-1.06249201
C	-3.57394275	-3.32609299	0.88586799
H	-1.84143875	-2.05194699	1.00464699
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H	-4.88269675	-0.87618399	-1.82125701

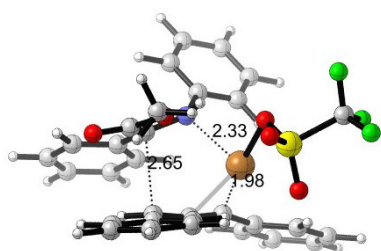
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H	-6.23202675	-2.87030999	-1.20052001
H	-5.39581075	-4.44462899	0.54963199
N	-2.51206975	-0.21988999	-0.89155801
H	-2.96184775	0.19433301	-1.70706601
Cu	1.79634725	0.74078901	-1.41501601
O	4.89795525	0.87998401	1.28959699
S	3.83863025	0.21261601	0.54799999
O	2.54710525	-0.03769099	1.22996699
O	3.63797725	0.75290201	-0.86565901
C	4.48264925	-1.50436999	0.17796099
F	5.72180325	-1.45506299	-0.29764701
F	4.47384025	-2.24643299	1.28802499
F	3.70052625	-2.10517799	-0.72994501



<b>E</b>			
C	-1.95979900	0.91815200	-0.02302400
C	-3.12470300	1.90297200	-0.22372600
C	-1.78650200	0.49059200	1.42418500
C	-2.89893600	0.25543400	2.24757500
C	-0.50004200	0.26649900	1.93398500
C	-2.72677100	-0.22020300	3.54710100
H	-3.90702000	0.43657100	1.87475600
C	-0.32931500	-0.21505800	3.23310300
H	0.38593300	0.47294600	1.33588600
C	-1.44106100	-0.46526300	4.04075600
H	-3.60109300	-0.40222400	4.17610200

H	0.68530500	-0.38355100	3.59972800
H	-1.30814900	-0.83987200	5.05863800
O	-3.56323500	1.87661200	-1.50457800
O	-3.55707400	2.65731200	0.60185500
C	-4.53125000	2.86937700	-1.86767500
H	-5.43646200	2.76368000	-1.25311400
H	-4.11172000	3.87386500	-1.71694400
H	-4.75750100	2.70076300	-2.92667600
C	-0.81162300	-0.65041100	-1.65250800
H	-1.09810700	-0.74084200	-2.71303000
C	-0.01164200	0.57837000	-1.41669800
C	-0.67016100	1.48105100	-0.64793300
C	-0.17948600	2.82715000	-0.28670700
C	-0.54863000	3.48546900	0.90184700
C	0.71865500	3.48587400	-1.15321700
C	-0.01786600	4.73737200	1.22041700
H	-1.24474700	3.01902700	1.59617300
C	1.25333700	4.72981900	-0.82905200
H	0.98913500	3.00356400	-2.09445100
C	0.88947600	5.36309400	0.36394200
H	-0.31261000	5.22062300	2.15495500
H	1.95519000	5.21073900	-1.51451700
H	1.30850800	6.33883000	0.62056300
C	-0.27651900	-1.98439100	-1.20459400
C	0.70020000	-2.09374200	-0.20706000
C	-0.79617100	-3.15242600	-1.78367500
C	1.12669500	-3.35198100	0.22257300
H	1.16011600	-1.20650400	0.22462400
C	-0.37442000	-4.40975700	-1.35212900
H	-1.55050800	-3.07536900	-2.57147500
C	0.58472400	-4.51075200	-0.33928200
H	1.90158300	-3.41620500	0.98880700
H	-0.79034700	-5.31091200	-1.80844500
H	0.92208700	-5.49366000	-0.00150900

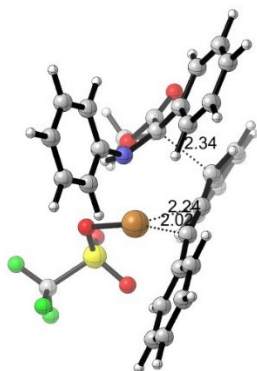
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C	-3.62532100	-3.23380600	0.88359800
H	-1.76474900	-2.14725900	0.98011400
C	-5.24191500	-2.46232700	-0.74300600
H	-4.64148800	-0.74575000	-1.91634400
C	-4.87391800	-3.35421000	0.26711400
H	-3.33167200	-3.92958000	1.67166800
H	-6.21521100	-2.54857700	-1.23021800
H	-5.56107500	-4.14582700	0.57360300
N	-2.22920200	-0.28054600	-0.96625200
H	-2.71884200	0.18234000	-1.73863000
Cu	1.87921400	0.67941200	-1.51558200
O	5.02717400	0.97532000	1.13512900
S	3.95559800	0.25832700	0.45857800
O	2.68735700	0.03779200	1.19155000
O	3.72424100	0.70991100	-0.97942500
C	4.60995400	-1.47204400	0.17589000
F	5.85661300	-1.43987600	-0.28317900
F	4.58975000	-2.16430800	1.31949900
F	3.84536400	-2.11924000	-0.71354500



<b>C'</b>			
C	1.71649800	1.19759600	0.88270200
C	1.01655000	2.48345400	1.10553900
C	3.11269900	1.09352000	0.46550300
C	4.00257800	2.18710800	0.55766000

C	3.59565300	-0.11630400	-0.08696600
C	5.32059200	2.06471700	0.12091700
H	3.64209200	3.12836700	0.96630300
C	4.91103700	-0.22358400	-0.52875400
H	2.93223700	-0.97208300	-0.18783500
C	5.78441900	0.86372500	-0.42442100
H	5.99364400	2.92082200	0.20910300
H	5.25795200	-1.16714900	-0.95677900
H	6.81839800	0.77509800	-0.76544000
O	-0.26832700	2.24429400	1.43229900
O	1.48882600	3.59637300	1.00130600
C	-1.15340700	3.35011100	1.64572000
H	-0.97043600	3.78394000	2.64073200
H	-0.99482100	4.11572500	0.87742700
H	-2.16236400	2.92885500	1.57514800
C	1.03660000	1.69628600	-1.62921600
H	2.07177000	2.04041900	-1.66721100
C	0.81753200	0.35507300	-1.83149400
C	0.60686900	-0.88242200	-1.84072200
C	0.58680300	-2.24479400	-2.30191300
C	-0.63913700	-2.93592100	-2.42706100
C	1.79252000	-2.92052200	-2.58060100
C	-0.64911100	-4.26873300	-2.83185300
H	-1.57393800	-2.41186300	-2.20984300
C	1.76804700	-4.25458400	-2.98428900
H	2.73860800	-2.38574600	-2.47812700
C	0.55110800	-4.93307000	-3.11002400
H	-1.60187100	-4.79362000	-2.93143400
H	2.70642000	-4.76983700	-3.20266800
H	0.53774300	-5.97898000	-3.42472700
C	-0.00879900	2.70156000	-1.70725300
C	-1.37909700	2.35690100	-1.70824900
C	0.34100400	4.06923300	-1.71572900
C	-2.35986200	3.34093000	-1.70414900

H	-1.68493500	1.31036300	-1.70130800
C	-0.64682300	5.05288800	-1.73477200
H	1.39526200	4.34991500	-1.69854700
C	-1.99900600	4.69506100	-1.72327300
H	-3.40912700	3.04275200	-1.66536200
H	-0.35911700	6.10675900	-1.74470400
H	-2.77098400	5.46811400	-1.72270900
C	1.60849000	-1.05921600	1.93255300
C	2.61357900	-0.88997900	2.89218500
C	1.14450600	-2.34110500	1.62563700
C	3.15707000	-2.00501500	3.52987200
H	2.96882300	0.11331600	3.13038700
C	1.68234200	-3.45288600	2.27608900
H	0.37133800	-2.47065200	0.86428900
C	2.69456200	-3.28886300	3.22482000
H	3.94410700	-1.86787900	4.27472900
H	1.31358400	-4.45045400	2.02849200
H	3.12273200	-4.15949000	3.72628300
N	1.01563700	0.08493200	1.28781000
H	0.11059100	0.34966800	1.69562000
Cu	-0.57608900	-0.58813200	-0.27747800
O	-3.75989100	1.30115300	0.77395000
S	-3.24943800	-0.02581200	0.43266300
O	-3.18957000	-0.41435300	-0.99406100
O	-1.93464800	-0.38951600	1.12673500
C	-4.42278600	-1.24046800	1.22198300
F	-4.48285800	-1.03649800	2.53443500
F	-5.63740400	-1.09259800	0.70203400
F	-4.00405800	-2.48644400	0.99611700



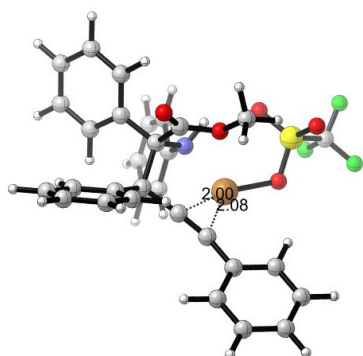
### TS5

C	1.94376600	0.95577500	0.59466100
C	1.50810200	2.33503700	0.94134100
C	3.33478900	0.62398900	0.23255300
C	4.39077800	1.54546900	0.37594900
C	3.62618600	-0.64707700	-0.30951200
C	5.69028900	1.19616200	0.00422500
H	4.18114500	2.53599300	0.77308400
C	4.92345800	-0.98426500	-0.68483100
H	2.82749800	-1.37333500	-0.44769300
C	5.96643100	-0.06608500	-0.52575600
H	6.49523700	1.92381000	0.13233900
H	5.12219200	-1.97378800	-1.10321900
H	6.98538100	-0.33318800	-0.81517700
O	0.23572200	2.30495700	1.37832300
O	2.14718700	3.35482100	0.80421500
C	-0.44980800	3.53879900	1.62488300
H	-0.13354500	3.95215500	2.59447700
H	-0.22646100	4.25866000	0.82827300
H	-1.51455900	3.27940400	1.62941800
C	1.27906100	1.33951700	-1.61493200
H	2.33018100	1.47810000	-1.87581600
C	0.76009300	0.06595100	-1.84745200
C	0.28971400	-1.08472300	-1.91061000
C	-0.14007800	-2.40864500	-2.26611000
C	-1.51808000	-2.72248300	-2.28347400



C	0.80613200	-3.41432500	-2.54898000
C	-1.92869400	-4.01890200	-2.58663700
H	-2.25124900	-1.94424500	-2.05406400
C	0.37966000	-4.70600400	-2.85292800
H	1.86942500	-3.16861000	-2.52736100
C	-0.98533000	-5.01227000	-2.87195200
H	-2.99494000	-4.25515200	-2.59944600
H	1.11743800	-5.48029900	-3.07558400
H	-1.31407100	-6.02680000	-3.10834500
C	0.42603600	2.52546800	-1.73149000
C	-0.97889400	2.44457300	-1.64582000
C	1.01861000	3.79616200	-1.87570300
C	-1.76346900	3.59216100	-1.68309700
H	-1.47334100	1.47809200	-1.54970300
C	0.22853000	4.94393900	-1.93415700
H	2.10549200	3.87587600	-1.93088700
C	-1.16304000	4.84839100	-1.83129500
H	-2.84556300	3.49579900	-1.57802700
H	0.70400900	5.92078800	-2.04876800
H	-1.77862500	5.75043400	-1.86339200
C	1.62614700	-1.20783900	1.81508300
C	2.66138800	-1.10330100	2.75170400
C	1.03853300	-2.45097400	1.56466100
C	3.10948100	-2.24136100	3.42231200
H	3.11766000	-0.13168300	2.94516400
C	1.48027000	-3.58614400	2.24732300
H	0.23909500	-2.53115100	0.82359900
C	2.52146700	-3.48540300	3.17294000
H	3.92096100	-2.15398600	4.14826200
H	1.01293800	-4.55216300	2.04461900
H	2.87444400	-4.37421900	3.70053000
N	1.12506400	-0.04083900	1.13307300
H	0.33843700	0.38706800	1.63309800
Cu	-0.65840800	-0.53092800	-0.21798500

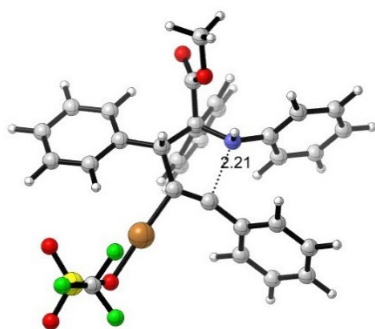
O	-3.40826700	1.91446500	0.90173300
S	-3.19439800	0.50833700	0.55919800
O	-3.30222300	0.10856300	-0.86073800
O	-1.94360000	-0.10185600	1.19375700
C	-4.54006400	-0.43947100	1.43383000
F	-4.48476600	-0.21837900	2.74377200
F	-5.72838300	-0.05442900	0.97750600
F	-4.39349000	-1.74591700	1.20858700



<b>F</b>			
C	-1.54689800	-0.49424500	-0.40965100
C	-1.19588900	0.12017600	-1.78112400
C	-2.70231200	-1.48602800	-0.52129700
C	-2.97279000	-2.15376900	-1.72506800
C	-3.41741600	-1.87423500	0.62236900
C	-3.93842200	-3.16047600	-1.78626200
H	-2.43735400	-1.88595700	-2.63475000
C	-4.38480200	-2.87797000	0.56412100
H	-3.20838000	-1.41494800	1.58736600
C	-4.65264100	-3.52496400	-0.64337400
H	-4.13288200	-3.65985200	-2.73814500
H	-4.92266200	-3.15974800	1.47206100
H	-5.40944300	-4.31122700	-0.69252700
O	0.12598500	0.23801400	-1.95031600
O	-2.01220900	0.49728000	-2.57920700
C	0.60258000	0.84943700	-3.16080900
H	0.13145900	0.37248500	-4.03069800

H	0.35133700	1.92002300	-3.15635900
H	1.68566000	0.68658300	-3.15263200
C	-1.86570200	0.73629900	0.55129600
H	-2.15441500	0.28665700	1.51174600
C	-0.61337500	1.49203300	0.77789100
C	0.31740600	2.31185100	0.87996000
C	1.12359700	3.49699400	0.98863300
C	2.50984600	3.44728500	0.74253500
C	0.51780300	4.72566900	1.32052300
C	3.27178700	4.61162400	0.82724100
H	2.97209000	2.49240800	0.48078700
C	1.29063700	5.88234200	1.40475600
H	-0.55747100	4.75872200	1.50637000
C	2.66710600	5.82827300	1.15916700
H	4.34569900	4.56791100	0.63302500
H	0.81714900	6.83246700	1.66277900
H	3.26930600	6.73734300	1.22649100
C	-3.00392500	1.63989800	0.09707200
C	-2.75818400	2.76481200	-0.70217500
C	-4.32252400	1.35846800	0.47766300
C	-3.80749900	3.58175400	-1.12345900
H	-1.73560700	3.00640100	-0.99592800
C	-5.37460900	2.17363700	0.05520900
H	-4.53459400	0.49386800	1.10699500
C	-5.12090800	3.28684400	-0.74904900
H	-3.59694000	4.45216600	-1.74907200
H	-6.39674900	1.93741800	0.36004900
H	-5.94343000	3.92565600	-1.07912100
C	-0.45452000	-2.06879200	1.23366400
C	-0.54447800	-3.44701500	1.00913200
C	-0.48486000	-1.57834600	2.54560700
C	-0.68235700	-4.32480400	2.08449500
H	-0.51072300	-3.82322300	-0.01471500
C	-0.64252000	-2.45803100	3.61856700

H	-0.36206400	-0.50891500	2.72713400
C	-0.74500500	-3.83309800	3.39150500
H	-0.74811700	-5.39917100	1.89873200
H	-0.66562200	-2.06643600	4.63813000
H	-0.85914800	-4.52087900	4.23227200
N	-0.31325100	-1.17056700	0.12425800
H	0.19735100	-1.64757200	-0.62842400
Cu	1.03216600	0.39719200	0.49526400
O	2.05375100	-2.11406400	-1.12364400
S	3.09657100	-1.07168900	-1.03140100
O	3.49094300	-0.39400600	-2.26953400
O	2.87965300	-0.11513100	0.13762500
C	4.61783300	-1.97685700	-0.45075900
F	4.36956500	-2.59945500	0.70004800
F	4.97238200	-2.88039200	-1.36171200
F	5.62401100	-1.12449600	-0.27292400

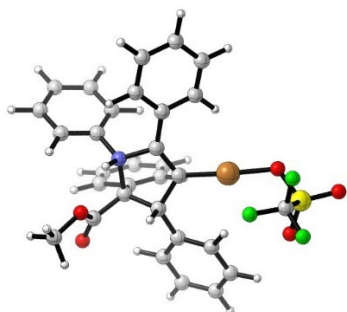


### TS6

C	-0.40049300	1.19641500	0.28599700
C	0.27004000	0.11368300	0.30049200
C	-0.26321500	-1.22662600	0.72311900
C	-1.83450800	-1.16600400	0.52612000
H	-2.06209600	0.20038500	2.02605300
N	-2.22590500	0.18607800	1.02061500
C	0.48645400	-2.42676800	0.14977000
C	1.89048000	-2.38356300	0.15419900
C	-0.14067800	-3.57227500	-0.35883900

C	2.65188500	-3.42637600	-0.37128500
H	2.42533400	-1.52947200	0.57682400
C	0.62169600	-4.62820200	-0.87045000
H	-1.22480400	-3.65847100	-0.37414900
C	2.01544500	-4.55745700	-0.88946000
H	3.73775800	-3.32101500	-0.38020100
H	0.11060900	-5.50776100	-1.26947400
H	2.60366400	-5.37775600	-1.30772700
C	-0.79536400	2.53280200	-0.02509500
C	-1.44074000	3.34631000	0.92667700
C	-0.58291100	3.03059800	-1.32851700
C	-1.86816400	4.62503700	0.57971300
H	-1.61576000	2.96024200	1.93162100
C	-0.99629500	4.31789800	-1.66114100
H	-0.08234600	2.39650200	-2.06235200
C	-1.64565700	5.11433700	-0.71163000
H	-2.37631400	5.24585700	1.32052600
H	-0.81703500	4.70043200	-2.66822700
H	-1.97830300	6.11991000	-0.97874500
C	-2.29508600	-1.35489100	-0.91310300
C	-1.44063200	-1.08686200	-1.99288400
C	-3.62538000	-1.70611800	-1.18532100
C	-1.90589000	-1.16189400	-3.30655800
H	-0.40022800	-0.81878800	-1.82163400
C	-4.09111500	-1.78469300	-2.49844500
H	-4.31371400	-1.91551000	-0.36841400
C	-3.23413900	-1.50901000	-3.56530300
H	-1.21999700	-0.95438100	-4.13089000
H	-5.13169000	-2.05924000	-2.68480000
H	-3.59671600	-1.57045800	-4.59406300
C	-2.44658500	-2.21715100	1.48485800
O	-2.94804800	-3.26530700	1.17863400
O	-2.31620700	-1.81512900	2.76570100
Cu	2.00192700	0.53376500	-0.39452300

O	4.77175500	-1.07380800	-0.24491000
S	4.95880400	0.35351100	-0.54084300
O	6.16519800	0.79169900	-1.22768400
O	3.69618700	1.01295000	-1.10532800
C	5.01879800	1.14595700	1.15291000
F	5.12604000	2.46955100	1.06536600
F	3.88133500	0.86406200	1.82334000
F	6.04226300	0.67486000	1.85789900
C	-3.48237900	0.78621100	0.73529600
C	-3.76586800	1.29868600	-0.53975800
C	-4.41645100	0.94855400	1.76864200
C	-4.97739300	1.94641400	-0.77276600
H	-3.03302800	1.19909200	-1.33750700
C	-5.62309900	1.61024300	1.53130500
H	-4.19201000	0.54852300	2.76087800
C	-5.90969800	2.10673300	0.25757200
H	-5.18843000	2.34140100	-1.76887200
H	-6.34208200	1.73226200	2.34463700
H	-6.85362600	2.62273000	0.06902900
H	-0.10814200	-1.25849000	1.81670200
C	-2.76318600	-2.73511900	3.76860400
H	-2.56233600	-2.25407300	4.73274300
H	-3.83756000	-2.93675800	3.65158900
H	-2.21363200	-3.68377400	3.68772400

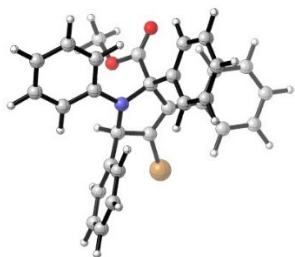


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C	-0.79373800	-1.13391400	-0.28268200
C	0.17927200	-0.21260000	-0.18897300

C	-0.32160600	1.11677100	-0.74661300
C	-1.87989600	1.01300600	-0.62953300
H	-2.07913500	-0.65105700	-1.86050600
N	-2.07915800	-0.52939400	-0.83914000
C	0.33642400	2.40174100	-0.25366300
C	1.73327700	2.42299700	-0.12301600
C	-0.37323500	3.58061200	0.01967800
C	2.40295600	3.56269300	0.32139700
H	2.33421800	1.54830700	-0.37265100
C	0.29704200	4.72940000	0.45102100
H	-1.45421300	3.62284300	-0.09852200
C	1.68356700	4.72311400	0.61652700
H	3.48640000	3.50988800	0.43996100
H	-0.27844000	5.63343700	0.66519500
H	2.20080200	5.61876900	0.96920200
C	-0.76831600	-2.58461700	-0.05526500
C	-1.53004900	-3.48271500	-0.82515800
C	0.07848300	-3.11265800	0.93868300
C	-1.44187000	-4.85993000	-0.61476700
H	-2.19508600	-3.11475000	-1.60893500
C	0.17087000	-4.48745600	1.14183800
H	0.66847300	-2.42697200	1.55046900
C	-0.59085400	-5.36959300	0.36800300
H	-2.03901400	-5.53775300	-1.22928900
H	0.84009200	-4.87183100	1.91488000
H	-0.52081200	-6.44732200	0.53105400
C	-2.45072900	1.40073900	0.71922100
C	-1.66703400	1.28874100	1.87865000
C	-3.79570800	1.77689500	0.84581400
C	-2.22160500	1.54096200	3.13337600
H	-0.61942200	1.00072600	1.80927400
C	-4.34867600	2.03141200	2.10101600
H	-4.42577900	1.87015600	-0.03737400
C	-3.56396000	1.91125800	3.24970000

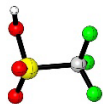
H	-1.59510500	1.45360900	4.02350500
H	-5.39822400	2.32300500	2.17871000
H	-3.99489900	2.11208900	4.23330700
C	-2.52947800	1.73144000	-1.81647100
O	-2.96437900	2.84948800	-1.80413900
O	-2.47031400	0.97326900	-2.93481800
Cu	1.92829700	-0.53544300	0.45804400
O	4.61491900	1.29395100	0.61867100
S	4.88493600	-0.14624100	0.73116700
O	6.08825200	-0.59313100	1.42062700
O	3.65249900	-0.95864900	1.13015100
C	5.09239000	-0.69743800	-1.04446800
F	5.29045200	-2.01217900	-1.12204400
F	3.98241200	-0.40218900	-1.74998000
F	6.12155200	-0.07366300	-1.61261900
C	-3.35744200	-1.05000200	-0.34334500
C	-3.48171100	-1.44734100	0.98637100
C	-4.44130100	-1.09099200	-1.21848400
C	-4.72231700	-1.88601600	1.44547800
H	-2.62152200	-1.40680700	1.65167700
C	-5.68086900	-1.53398200	-0.74948500
H	-4.32104900	-0.77613600	-2.25667400
C	-5.82223200	-1.92826700	0.58273000
H	-4.82852700	-2.19584600	2.48674000
H	-6.53432700	-1.57091500	-1.42945700
H	-6.79095600	-2.27401300	0.94948600
H	-0.09059400	1.05886800	-1.82846800
C	-2.89268300	1.60002200	-4.15605000
H	-2.76212300	0.84811600	-4.94222700
H	-3.94447600	1.90948500	-4.08060500
H	-2.27316700	2.48473500	-4.35805500





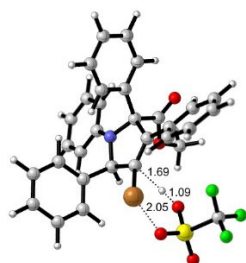
H			
C	-0.41622000	-0.92120500	-0.24035200
C	-0.62619100	-1.77845000	-1.51688700
C	-0.91321600	-1.53854300	1.07728700
C	-1.55079900	-2.77837400	1.20738400
C	-0.72415900	-0.75987900	2.22973200
C	-1.96878500	-3.23180000	2.46370700
H	-1.72785200	-3.39054800	0.32642600
C	-1.14133600	-1.21036200	3.48047300
H	-0.25150300	0.21785700	2.13520200
C	-1.76589000	-2.45551300	3.60433800
H	-2.46088700	-4.20434500	2.54344100
H	-0.98212100	-0.58466600	4.36219400
H	-2.09545800	-2.81335000	4.58275300
O	0.19269200	-1.36178200	-2.48995700
O	-1.43478100	-2.66140200	-1.68583100
C	0.10944400	-2.05892300	-3.73034200
H	0.34517700	-3.12384700	-3.58777700
H	-0.90098600	-1.97514600	-4.15763000
H	0.84813800	-1.59073100	-4.39130700
C	1.18112000	0.85256100	-0.65205400
H	1.62466500	0.83585000	-1.66901500
C	-0.22565700	1.39965700	-0.72953000
C	-1.12874800	0.43575400	-0.47273200
C	-2.58892800	0.60367300	-0.33059600
C	-3.50714200	-0.40854300	-0.66800300
C	-3.10553500	1.81363400	0.17560600
C	-4.88188500	-0.19822500	-0.54154900

H	-3.15058300	-1.36710100	-1.04017000
C	-4.47772400	2.02578500	0.29508100
H	-2.40702000	2.58284100	0.51495100
C	-5.37699600	1.01912300	-0.06890200
H	-5.57226400	-0.99933700	-0.81692600
H	-4.84701700	2.97313000	0.69645700
H	-6.45344400	1.17719100	0.03160800
C	2.05449700	1.73560200	0.22804000
C	2.30922000	1.43217900	1.56868900
C	2.57025400	2.92563400	-0.30738400
C	3.05231800	2.30929800	2.36442800
H	1.93395700	0.49453400	1.97942700
C	3.30915300	3.80582300	0.48625500
H	2.40044100	3.15410800	-1.36421400
C	3.54922000	3.50082100	1.82992100
H	3.24814900	2.05585600	3.40929800
H	3.70742400	4.72727900	0.05368300
H	4.13072600	4.18417500	2.45332400
C	2.02800000	-1.44218300	-0.24099600
C	1.80627900	-2.81493700	0.00581100
C	3.33999600	-1.04065100	-0.57678100
C	2.85063400	-3.73491600	-0.08083200
H	0.81839400	-3.17043600	0.28598100
C	4.37485700	-1.97243500	-0.65459700
H	3.56175100	0.00689600	-0.76891800
C	4.14575200	-3.32827600	-0.41021600
H	2.64056600	-4.78900900	0.11844100
H	5.37820800	-1.62485900	-0.91471000
H	4.96006300	-4.05301400	-0.47372300
N	0.99375700	-0.51087500	-0.16269900
Cu	-0.53301100	3.23863100	-0.98391700



**CF<sub>3</sub>SO<sub>3</sub>H**

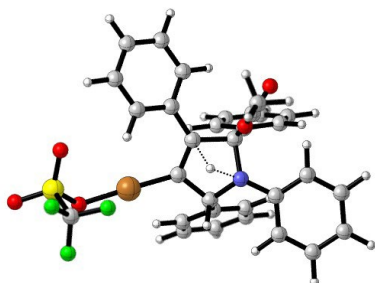
O	-1.24876500	0.21590500	1.43459300
S	-0.86045900	-0.14477500	0.08202300
O	-1.23067100	-1.37503700	-0.57687900
O	-1.24630700	1.07552900	-0.92186700
C	1.00573200	0.00159100	-0.00305800
F	1.42736500	-0.25588200	-1.22955800
F	1.35628000	1.23917100	0.33909600
F	1.53832000	-0.86217600	0.84732500
H	-1.35878800	1.88564300	-0.39255800

**TS7**

C	1.59305300	0.92307400	0.34091600
C	1.50938200	1.41581700	1.81248600
C	2.43719200	1.77105900	-0.62199000
C	3.01846000	3.00855300	-0.31923700
C	2.57877200	1.26331700	-1.92314200
C	3.74064700	3.70694900	-1.29366500
H	2.90894000	3.42691100	0.67801000
C	3.29548200	1.96073700	-2.89337700
H	2.11312100	0.30974200	-2.17227100
C	3.88509000	3.18971600	-2.58076000
H	4.19189200	4.66837000	-1.03614900
H	3.39239900	1.54403700	-3.89894500
H	4.44906500	3.74002900	-3.33769700
O	1.04020500	0.43062900	2.58659900
O	1.75089900	2.52011000	2.23916000
C	0.88033400	0.72662400	3.97298600

H	1.85093300	0.98066300	4.42359400
H	0.19166000	1.57299600	4.11198000
H	0.47143400	-0.18152800	4.43035800
C	0.83389300	-1.36816600	0.17937900
H	0.58405400	-1.84427700	1.14977200
C	-0.28974500	-0.43910100	-0.23919100
C	0.14426100	0.84124400	-0.18950700
C	-0.62340700	2.01688200	-0.63220700
C	-0.54503700	3.26683800	0.01164500
C	-1.48400800	1.89775900	-1.74193200
C	-1.33451700	4.33593000	-0.41355000
H	0.12608200	3.40434900	0.85791500
C	-2.27559000	2.96450200	-2.16277300
H	-1.49454100	0.95571600	-2.29740600
C	-2.20823000	4.18994400	-1.49468800
H	-1.26496000	5.29381600	0.10742000
H	-2.93368700	2.84470000	-3.02683000
H	-2.82074300	5.03197000	-1.82562000
C	0.96875000	-2.46492400	-0.86726100
C	2.01266700	-2.50474100	-1.79450700
C	-0.05883400	-3.42241900	-0.95801200
C	2.02410200	-3.47238100	-2.80520200
H	2.82037400	-1.77657700	-1.71580300
C	-0.05107100	-4.38529500	-1.97085200
H	-0.85690700	-3.42854100	-0.20815900
C	0.99144100	-4.40813800	-2.90342700
H	2.84930200	-3.49368500	-3.52129600
H	-0.85487500	-5.12361800	-2.02569600
H	1.00292500	-5.15991600	-3.69590300
C	3.13147700	-0.92456900	1.00602500
C	4.15681000	-0.02488100	1.37042500
C	3.29587400	-2.28444400	1.34890400
C	5.29023100	-0.47268300	2.04856500
H	4.08349300	1.02793700	1.10901700

C	4.43795200	-2.71717300	2.02244900
H	2.53433000	-3.01440800	1.08143800
C	5.44629300	-1.82013900	2.38208300
H	6.06456000	0.25141600	2.31468700
H	4.53382000	-3.77733500	2.27104800
H	6.33727300	-2.16479000	2.91087400
N	1.99023200	-0.49256600	0.33089600
Cu	-1.77961000	-1.21947800	-1.21819700
O	-3.62873000	-1.67126500	-0.45192300
S	-3.77609400	-1.19910700	0.95759900
O	-4.50665400	-2.01956900	1.89443800
C	-4.66269300	0.44189800	0.80896300
F	-3.93688600	1.26227900	0.06093300
F	-5.84016000	0.23809300	0.23674700
F	-4.83109800	0.96223100	2.01311400
O	-2.39409500	-0.75281200	1.53727300
H	-1.63925800	-0.58033100	0.76670600

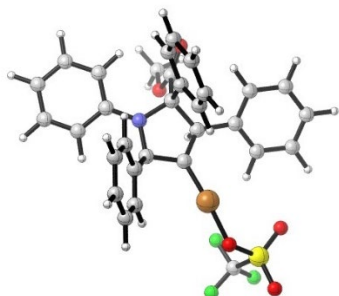


### TS8

C	0.86221000	-1.22014400	0.47971200
C	-0.25199100	-0.35814700	-0.08664700
C	0.24878900	0.93307200	-0.23512400
C	1.77174500	0.98495700	0.06102600
H	0.46058900	-1.78939500	1.33018700
N	1.74325200	-0.15681300	1.05469700
C	-0.50019900	2.09192100	-0.75372100
C	-1.89183000	2.16788900	-0.56313800
C	0.14091100	3.11029100	-1.48476900

C	-2.63106100	3.21208900	-1.11147200
H	-2.41814200	1.40994000	0.01640200
C	-0.60210000	4.16330000	-2.02245700
H	1.21590600	3.07404100	-1.66036100
C	-1.98713700	4.21572200	-1.84250300
H	-3.71284500	3.21439100	-0.96830500
H	-0.09250400	4.94070700	-2.59634600
H	-2.56468200	5.03645400	-2.27456500
C	1.47016500	-2.19478100	-0.52031400
C	2.85133600	-2.33995700	-0.69878900
C	0.60307000	-2.99885100	-1.27631400
C	3.35350900	-3.24511800	-1.63553700
H	3.54933100	-1.73075100	-0.12962300
C	1.10563700	-3.90688600	-2.20921000
H	-0.47657400	-2.90221700	-1.14339600
C	2.48480800	-4.02914700	-2.39712300
H	4.43389100	-3.32867700	-1.77197800
H	0.41304500	-4.51629700	-2.79411900
H	2.87972400	-4.73363600	-3.13272500
C	2.65683900	0.76010400	-1.15243700
C	2.09260300	0.35189000	-2.36932900
C	4.05203900	0.88241900	-1.06420900
C	2.90134700	0.03995200	-3.46250100
H	1.01137400	0.25696300	-2.46615100
C	4.86094600	0.56578800	-2.15551400
H	4.51827100	1.22260200	-0.14277600
C	4.28940100	0.13726600	-3.35675100
H	2.44038300	-0.28771900	-4.39643000
H	5.94558900	0.65971600	-2.06649000
H	4.92492900	-0.11180200	-4.20964400
C	2.05423700	2.31477400	0.79252200
O	2.80733400	3.17076100	0.40861600
O	1.30164100	2.41136300	1.89119900
Cu	-2.01351800	-0.92729200	-0.42085100

O	-4.70023700	0.79710900	-0.58397800
S	-4.96720700	-0.62472400	-0.32264600
O	-6.24664600	-1.19726700	-0.71531000
O	-3.78683200	-1.52906800	-0.69195700
C	-4.90761000	-0.74744100	1.54315100
F	-5.06521500	-2.00428500	1.95122400
F	-3.71048100	-0.31245800	1.98912900
F	-5.85323700	0.00764500	2.09407400
C	2.78880800	-0.48304900	1.96706100
C	3.78213700	0.44081700	2.33044900
C	2.80385500	-1.75395200	2.57065400
C	4.75760900	0.10033600	3.26927100
H	3.82608500	1.43078900	1.88681900
C	3.78084100	-2.08267200	3.50884000
H	2.06405700	-2.50490700	2.30124500
C	4.76543600	-1.15975500	3.86791400
H	5.52028400	0.83787100	3.52906100
H	3.77011700	-3.07836300	3.95759800
H	5.53053600	-1.42135200	4.60132900
H	0.41572100	0.48228500	1.24055600
C	1.37704900	3.64072500	2.62017400
H	0.67334500	3.54096200	3.45386700
H	2.39931000	3.79997800	2.99324700
H	1.09473700	4.48138800	1.97086400

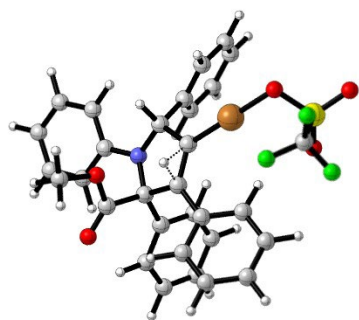


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C	0.87066700	-1.15966700	0.56789200
C	-0.18805100	-0.17598800	0.21620600

C	0.38386800	1.15762900	0.43388700
C	1.92919700	0.97771900	0.25416600
H	0.53019900	-1.62375800	1.52012600
N	2.08826900	-0.39694900	0.76151600
C	-0.33130700	2.38245200	-0.09498800
C	-1.72973000	2.43523500	-0.00097000
C	0.35035100	3.46618100	-0.66677700
C	-2.44312300	3.51968400	-0.50924400
H	-2.29571100	1.62938600	0.46869700
C	-0.36395000	4.56266200	-1.15843200
H	1.43606900	3.46437100	-0.74677100
C	-1.75879500	4.58995700	-1.09160400
H	-3.53252800	3.50070200	-0.45078500
H	0.18105700	5.39630700	-1.60731500
H	-2.31136100	5.44334200	-1.49167500
C	0.92057700	-2.28022700	-0.48240000
C	1.97135400	-2.37041800	-1.39743300
C	-0.13275900	-3.20291800	-0.54092000
C	1.96416200	-3.37491700	-2.36943600
H	2.79467800	-1.65890400	-1.35447800
C	-0.14196300	-4.20057900	-1.51643000
H	-0.95375800	-3.14537100	0.17981200
C	0.90841200	-4.28666600	-2.43590700
H	2.79064000	-3.43843900	-3.08069100
H	-0.97120400	-4.91007100	-1.55745300
H	0.90316600	-5.06610500	-3.20117500
C	2.33177600	1.04886900	-1.22116800
C	1.38858100	0.70905400	-2.20461700
C	3.65191200	1.29470100	-1.62879300
C	1.75106000	0.58332800	-3.54496700
H	0.34181100	0.53963900	-1.94013700
C	4.01728900	1.17232300	-2.97127600
H	4.40182300	1.60052700	-0.90434500
C	3.07225700	0.81107000	-3.93432100



H	0.99437600	0.31208500	-4.28389300
H	5.05171300	1.36615400	-3.26403900
H	3.36116900	0.71891500	-4.98371900
C	2.61807400	2.01046200	1.16697400
O	3.29611500	2.93523500	0.79714300
O	2.31350400	1.77437200	2.44625100
Cu	-1.90634000	-0.62650600	-0.29769700
O	-4.57428300	1.10800600	-0.32621800
S	-4.86049400	-0.33085000	-0.26556700
O	-6.11633100	-0.84468500	-0.78781700
O	-3.65723600	-1.18621300	-0.70083500
C	-4.86514000	-0.71071800	1.56634600
F	-5.05554200	-2.00741000	1.78985500
F	-3.67164200	-0.36702000	2.09748700
F	-5.81141500	-0.01735300	2.18728700
C	3.24403700	-0.97149600	1.28300400
C	4.47440900	-0.28522500	1.34263600
C	3.20465300	-2.29075900	1.78778400
C	5.60310500	-0.88669600	1.89998300
H	4.57212500	0.72063400	0.94596500
C	4.34126700	-2.87958500	2.33888500
H	2.28587900	-2.87312300	1.74158800
C	5.55226000	-2.18678600	2.40532900
H	6.53863100	-0.32253700	1.92915400
H	4.27287100	-3.90179900	2.71904600
H	6.43998000	-2.65405600	2.83553200
H	0.25491000	1.14723800	1.54879200
C	2.90032700	2.64961300	3.41411500
H	2.51434000	2.32672900	4.38746600
H	3.99597300	2.55855300	3.38750700
H	2.62161600	3.69307000	3.20946800

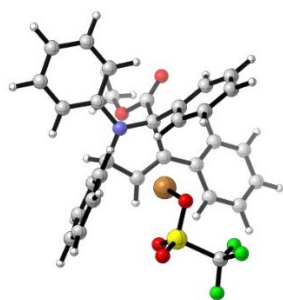


**TS9**

C	-1.17926100	-1.33677300	-0.63868000
C	0.03817900	-0.44882700	-0.54320800
C	-0.41528200	0.87551600	-0.34689300
C	-1.95816400	0.93088900	-0.21730200
H	-1.25790200	-1.71363200	-1.67868100
N	-2.31437900	-0.48929700	-0.30300400
C	0.44711200	2.04096500	-0.03270100
C	1.67545700	1.83542900	0.61393100
C	0.06294400	3.34800100	-0.38302200
C	2.52600600	2.90948100	0.87238600
H	1.98439900	0.84158400	0.93689800
C	0.91216600	4.41999700	-0.11454300
H	-0.89596100	3.53733000	-0.86524400
C	2.14792700	4.20272600	0.50628100
H	3.48343000	2.71588700	1.35972200
H	0.60866900	5.43139900	-0.39339200
H	2.81153600	5.04651300	0.70967900
C	-0.97608400	-2.53927300	0.28249900
C	-1.68599500	-2.68289400	1.47763100
C	-0.02078000	-3.50479400	-0.06955400
C	-1.43509700	-3.77356100	2.31662500
H	-2.44409300	-1.94723400	1.74528400
C	0.23495400	-4.58793400	0.77115100
H	0.53036200	-3.40807500	-1.00936900
C	-0.47176600	-4.72302900	1.97069100
H	-1.99866500	-3.87836300	3.24660000

H	0.99014800	-5.32517100	0.49031800
H	-0.27187000	-5.56931700	2.63169100
C	-2.28488300	1.54455600	1.15113500
C	-1.78031500	0.85795300	2.26729200
C	-2.98507500	2.73991100	1.35586700
C	-1.98009700	1.34243900	3.55828100
H	-1.21674900	-0.06474600	2.12785700
C	-3.19070200	3.22062000	2.65356400
H	-3.37472800	3.29404000	0.50642500
C	-2.69256300	2.52862000	3.75738400
H	-1.57315900	0.79295800	4.41003700
H	-3.74602100	4.15075700	2.79532500
H	-2.85268000	2.91210900	4.76763000
C	-2.51879400	1.65666100	-1.47446200
O	-3.17213700	2.66527200	-1.53219100
O	-2.13923400	0.96963500	-2.56454000
Cu	1.81251900	-1.09043500	-0.57654000
O	3.82717400	-0.34277900	1.41821600
S	4.55439000	-1.01610700	0.32565700
O	5.75631900	-1.77672900	0.62949500
O	3.59518100	-1.75358400	-0.61612100
C	5.10438400	0.38818600	-0.78319500
F	5.89000100	-0.05204900	-1.75961200
F	4.03325000	0.98268600	-1.33672900
F	5.76468700	1.30370800	-0.07380800
C	-3.62425100	-0.90017900	-0.57075600
C	-4.72016200	-0.04639000	-0.32796700
C	-3.88345000	-2.18769300	-1.08566200
C	-6.02068100	-0.46511500	-0.60976200
H	-4.56637600	0.93997800	0.10259900
C	-5.19055800	-2.59305000	-1.35548800
H	-3.06882800	-2.88806100	-1.26097900
C	-6.27085700	-1.73796800	-1.12712400
H	-6.84904400	0.21924200	-0.41098300

H	-5.36059500	-3.59728200	-1.75145600
H	-7.29136500	-2.06116500	-1.34161500
C	-2.63269300	1.43973000	-3.82401300
H	-2.22163900	0.76288000	-4.58124100
H	-3.73128000	1.40585100	-3.83158700
H	-2.30363400	2.47294600	-4.00535700
H	-0.13617500	0.50615400	-1.51983000



**CuOTf + 3b**

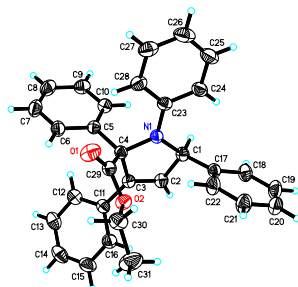
C	1.24479000	1.21310000	-1.36293000
C	0.35841700	0.04715200	-1.72336100
C	0.64091300	-1.06673200	-0.97526900
C	1.85275200	-0.76753700	-0.06799500
H	1.93068400	1.43838200	-2.20377300
N	1.98150600	0.69452700	-0.21202700
C	0.01114600	-2.39632400	-1.14135000
C	-1.35191600	-2.47806100	-1.49753400
C	0.72695300	-3.59235300	-0.96423500
C	-1.97520700	-3.71140600	-1.66612700
H	-1.94797100	-1.56813300	-1.61051800
C	0.10029500	-4.82759400	-1.14340800
H	1.78068900	-3.57154000	-0.69667700
C	-1.25006800	-4.89438900	-1.49091900
H	-3.03712300	-3.74441700	-1.91845400
H	0.67654300	-5.74491400	-1.00309700
H	-1.73931500	-5.86298500	-1.61571000
C	0.35180300	2.42039200	-1.07840200
C	0.05054800	2.82643500	0.22836700

C	-0.32866300	3.01725000	-2.14839700
C	-0.95701700	3.76605100	0.46308500
H	0.61071200	2.40982000	1.06439500
C	-1.32918600	3.95987600	-1.91404900
H	-0.09963400	2.71177600	-3.17349200
C	-1.66192600	4.32012500	-0.60532200
H	-1.20674600	4.04498000	1.48830700
H	-1.87203200	4.39486300	-2.75606500
H	-2.47535000	5.02313100	-0.41791400
C	1.53410300	-1.20900600	1.36983700
C	0.68106800	-0.38319900	2.11755600
C	1.92509700	-2.43490600	1.92651700
C	0.20513700	-0.77097300	3.36911400
H	0.38797400	0.58755300	1.72412300
C	1.46243200	-2.81715300	3.18997700
H	2.60487600	-3.08721800	1.38758600
C	0.59547200	-1.99656800	3.91279300
H	-0.47720500	-0.11098600	3.90799500
H	1.78268200	-3.77567000	3.60527200
H	0.22684800	-2.30887600	4.89252100
C	3.11476900	-1.42138800	-0.71252900
O	3.80199300	-2.30276100	-0.26182700
O	3.35043000	-0.84745800	-1.89781400
Cu	-0.99968900	0.13106700	-0.15822300
O	-2.36029500	0.54338100	1.30655900
S	-3.43122100	1.09938200	0.38314900
O	-4.09056200	2.32194700	0.81617900
O	-2.90133400	1.02600100	-1.01723800
C	-4.73085100	-0.23904000	0.42534600
F	-5.73186800	0.06788000	-0.39436700
F	-4.19151400	-1.39874600	0.02746300
F	-5.20617200	-0.38928000	1.65656300
C	3.12845900	1.35808000	0.24215700
C	3.98807900	0.76974400	1.19319400

C	3.45085400	2.64366700	-0.24040400
C	5.12537700	1.44624100	1.63471100
H	3.76868700	-0.21280300	1.60448200
C	4.58860500	3.30907300	0.21627000
H	2.80484500	3.14018300	-0.96206100
C	5.43860100	2.71956900	1.15435100
H	5.77155500	0.96330300	2.37181900
H	4.80897800	4.30606600	-0.17329600
H	6.32829700	3.24485400	1.50728200
C	4.51573800	-1.28923300	-2.59821500
H	4.54191100	-0.71745700	-3.53278400
H	5.41627900	-1.09002900	-1.99965000
H	4.45670100	-2.36772500	-2.80510000
H	-0.29821400	0.07217100	-2.59368300

## 7. X-Ray crystallographic studies

Single crystal for the X-ray diffraction studies for compounds **3a** was carried out on a SMART APEX diffractometer with graphite-monochromated Mo radiation ( $\lambda = 0.71073 \text{ \AA}$ ). Cell parameters were obtained by global refinement of the positions of all collected reflections. Intensities were corrected for Lorentz and polarization effects and empirical absorption. The structures were solved by direct methods and refined by full-matrix least squares on  $F^2$ . All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in calculated positions. Structure solution and refinement were performed by using the SHELXL-97 package. The X-ray crystallographic files, in CIF format, are available from the Cambridge Crystallographic Data Centre on quoting the deposition numbers CCDC 2314497 for **3a**. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44-1223-336033; e-mail: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk) or [www: http://www.ccdc.cam.ac.uk](http://www.ccdc.cam.ac.uk)).

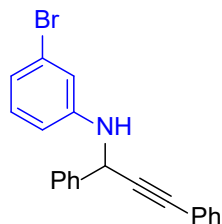


**Figure S3.** Molecular structure of compound **3a**.

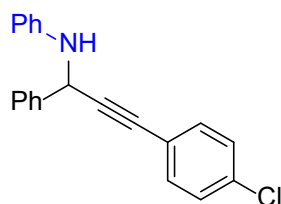
**Table S2.** Crystal data and structure refinement for **3a**

Empirical formula	C <sub>31</sub> H <sub>27</sub> NO <sub>2</sub>	
Formula weight	445.53	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 27.8591(8) Å	α = 90°
	b = 9.4831(3) Å	β = 105.0080(10)°
	c = 19.0167(6) Å	γ = 90°
Volume	4852.7(3) Å <sup>3</sup>	
Z	8	
Density (calculated)	1.220 Mg/m <sup>3</sup>	
Absorption coefficient	0.075 mm <sup>-1</sup>	
F(000)	1888	
Crystal size	0.200 x 0.160 x 0.130 mm <sup>3</sup>	
Theta range for data collection	2.992 to 25.999°.	
Index ranges	-34 ≤ h ≤ 34, -11 ≤ k ≤ 11, -23 ≤ l ≤ 23	
Reflections collected	29026	
Independent reflections	4749 [R(int) = 0.0728]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5000	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	4749 / 0 / 308	
Goodness-of-fit on F <sup>2</sup>	1.028	
Final R indices [I > 2σ(I)]	R1 = 0.0470, wR2 = 0.1160	
R indices (all data)	R1 = 0.0470, wR2 = 0.1160	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.198 and -0.143 e.Å <sup>-3</sup>	

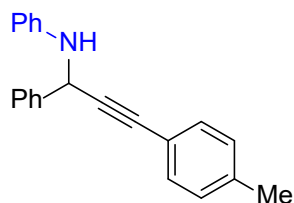
## 8. Analytical data



**3-Bromo-*N*-(1,3-diphenylprop-2-yn-1-yl)aniline (1u):** 1.91 g, yield 53%, yellow solid. M.p.: 98.5-98.3 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 7.4$  Hz, 2H), 7.51 – 7.45 (m, 4H), 7.41 (t,  $J = 7.3$  Hz, 1H), 7.37 – 7.31 (m, 3H), 7.10 (t,  $J = 8.0$  Hz, 1H), 7.00 (t,  $J = 2.1$  Hz, 1H), 6.96 (d,  $J = 7.8$  Hz, 1H), 6.72 (dd,  $J = 8.1, 1.4$  Hz, 1H), 5.52 (s, 1H), 4.26 (s, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  147.8, 139.2, 131.9, 130.5, 129.0, 128.6, 128.4, 128.4, 127.4, 123.2, 122.6, 121.4, 116.9, 112.7, 87.8, 85.5, 50.5. HRMS calcd for  $\text{C}_{21}\text{H}_{16}\text{BrN}$  [ $\text{M}+\text{H}$ ] $^+$ : 362.0539; Found: 362.0538.



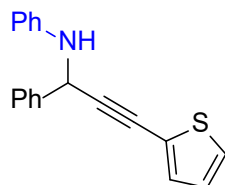
***N*-(3-(4-Chlorophenyl)-1-phenylprop-2-yn-1-yl)aniline (1z6):** 2.06 g, yield 65%, yellow solid. M.p.: 106.4-107.3 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (d,  $J = 7.7$  Hz, 2H), 7.45 (t,  $J = 7.2$  Hz, 2H), 7.41 – 7.34 (m, 3H), 7.31 – 7.23 (m, 4H), 6.87 – 6.78 (m, 3H), 5.53 (s, 1H), 4.18 (s, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  146.6, 139.6, 134.4, 133.1, 129.3, 129.0, 128.7, 128.3, 127.4, 121.4, 118.8, 114.2, 89.6, 84.1, 50.7. HRMS calcd for  $\text{C}_{21}\text{H}_{16}\text{ClN}$  [ $\text{M}+\text{H}$ ] $^+$ : 318.1044; Found: 318.1051.



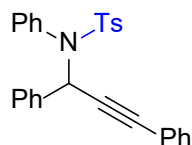
***N*-(1-Phenyl-3-(*p*-tolyl)prop-2-yn-1-yl)aniline (1z7):** 1.81 g, yield 61%, yellow solid. M.p.: 99.5-102.1 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 7.5$  Hz, 2H), 7.43 (t,  $J = 7.3$  Hz, 2H), 7.39 – 7.30 (m, 3H), 7.24 (t,  $J = 7.9$  Hz, 2H), 7.11 (d,  $J = 7.9$  Hz, 2H),



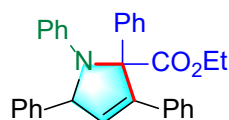
6.82 (t,  $J = 8.4$  Hz, 3H), 5.52 (s, 1H), 4.23 (s, 1H), 2.35 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  146.7 140.0, 138.5, 131.8, 129.3, 129.1, 128.9, 128.2, 127.4, 119.8, 118.7, 114.2, 87.8, 85.3, 50.8, 21.6. HRMS calcd for  $\text{C}_{22}\text{H}_{19}\text{N}$   $[\text{M}+\text{H}]^+$ : 298.1509; Found: 298.1508.



***N*-(1-Phenyl-3-(thiophen-2-yl)prop-2-yn-1-yl)aniline (1z8)**: 1.41 g, yield 49%, gray solid. M.p.: 86.7-89.1 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 7.4$  Hz, 2H), 7.48 (t,  $J = 7.4$  Hz, 2H), 7.42 (t,  $J = 7.3$  Hz, 1H), 7.33 – 7.23 (m, 4H), 7.00 (dd,  $J = 5.1, 3.7$  Hz, 1H), 6.88 (t,  $J = 7.4$  Hz, 1H), 6.84 (d,  $J = 7.4$  Hz, 2H), 5.59 (s, 1H), 4.23 (s, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  146.5, 139.5, 132.3, 129.3, 128.9, 128.3, 127.4, 127.2, 127.0, 122.5, 118.7, 114.1, 92.5, 78.4, 50.9. HRMS calcd for  $\text{C}_{19}\text{H}_{15}\text{NS}$   $[\text{M}+\text{H}]^+$ : 290.0998; Found: 290.0983.

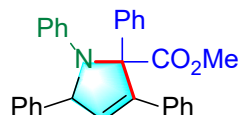


***N*-(1,3-Diphenylprop-2-yn-1-yl)-4-methyl-N-phenylbenzenesulfonamide (1a')**: 175 mg, yield 81%, white solid. M.p.: 310.1-312.5 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.2$  Hz, 2H), 7.48 – 7.40 (m, 2H), 7.38 – 7.28 (m, 3H), 7.27 – 7.23 (m, 7H), 7.23 – 7.18 (m, 1H), 7.13 (t,  $J = 8.7$  Hz, 2H), 6.95 (d,  $J = 8.3$  Hz, 2H), 6.74 (s, 1H), 2.40 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.5, 137.0, 136.3, 136.0, 131.8, 131.6, 129.4, 128.8, 128.7, 128.5, 128.4, 128.4, 128.3, 122.4, 88.5, 85.4, 55.8, 21.7. HRMS calcd for  $\text{C}_{28}\text{H}_{23}\text{NO}_2\text{S}$   $[\text{M}+\text{Na}]^+$ : 460.1342; Found: 460.1346.

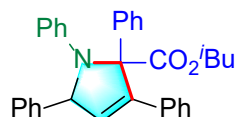


**Ethyl 1,2,3,5-tetraphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3a)**: 147 mg, yield 68%, white solid. M.p.: 281.7-283.1 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 (d,  $J$

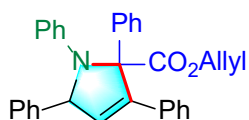
= 7.2 Hz, 2H), 7.59 (d,  $J = 7.5$  Hz, 2H), 7.42 (t,  $J = 7.5$  Hz, 2H), 7.37 – 7.24 (m, 3H), 7.26 – 7.17 (m, 4H), 7.06 – 6.95 (m, 4H), 6.61 (d,  $J = 9.0$  Hz, 3H), 6.20 (d,  $J = 2.1$  Hz, 1H), 6.06 (d,  $J = 2.2$  Hz, 1H), 4.38 (q,  $J = 7.1$  Hz, 2H), 1.28 (t,  $J = 7.1$  Hz, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.8, 143.4, 143.2, 141.2, 138.6, 133.6, 129.7, 128.8, 128.6, 128.3, 128.1, 128.0, 127.9, 127.5, 127.4, 127.0, 117.2, 115.5, 81.3, 71.2, 61.8, 14.1. HRMS calcd for  $\text{C}_{31}\text{H}_{27}\text{NO}_2$  [ $\text{M}+\text{Na}$ ] $^+$ : 468.1934; Found: 468.1932.



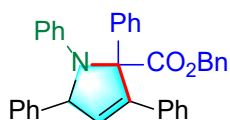
**Methyl 1,2,3,5-tetraphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3b):** 145 mg, yield 65%, white solid. M.p.: 273.1-275.1 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64 (d,  $J = 7.0$  Hz, 2H), 7.53 (d,  $J = 7.0$  Hz, 2H), 7.40 (t,  $J = 7.6$  Hz, 2H), 7.30 (t,  $J = 7.3$  Hz, 1H), 7.27 – 7.15 (m, 6H), 6.98 (t,  $J = 8.0$  Hz, 4H), 6.62 – 6.53 (m, 3H), 6.17 (d,  $J = 2.2$  Hz, 1H), 6.04 (d,  $J = 2.2$  Hz, 1H), 3.87 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 143.3, 143.2, 141.1, 138.4, 133.4, 129.7, 129.0, 128.6, 128.4, 128.2, 128.14, 128.08, 128.0, 127.6, 127.5, 126.9, 117.3, 115.5, 81.3, 71.3, 52.6. HRMS calcd for  $\text{C}_{30}\text{H}_{25}\text{NO}_2$  [ $\text{M}+\text{Na}$ ] $^+$ : 454.1778; Found: 454.1788.



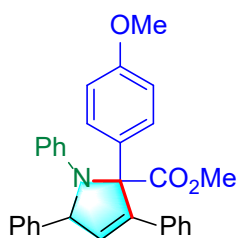
**Isobutyl 1,2,3,5-tetraphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3c):** 128 mg, yield 57%, white solid. M.p.: 210.3-212.4 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 6.9$  Hz, 2H), 7.61 (d,  $J = 7.1$  Hz, 2H), 7.41 (t,  $J = 7.5$  Hz, 2H), 7.35 – 7.27 (m, 3H), 7.27 – 7.21 (m, 2H), 7.19 (t,  $J = 7.2$  Hz, 2H), 7.03 – 6.95 (m, 4H), 6.64 – 6.56 (m, 3H), 6.23 (d,  $J = 2.2$  Hz, 1H), 6.05 (d,  $J = 2.2$  Hz, 1H), 4.17 – 4.02 (m, 2H), 2.00 – 1.86 (m, 1H), 0.84 (d,  $J = 6.7$  Hz, 6H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.0, 143.2, 143.1, 141.3, 138.7, 133.7, 129.9, 128.9, 128.6, 128.22, 128.17, 128.09, 128.05, 128.0, 127.6, 127.4, 126.9, 117.2, 115.6, 81.5, 72.3, 71.1, 27.7, 19.3, 19.2. HRMS calcd for  $\text{C}_{33}\text{H}_{31}\text{NO}_2$  [ $\text{M}+\text{Na}$ ] $^+$ : 496.2247; Found: 496.2264.



**Allyl 1,2,3,5-tetraphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3d):** 150 mg, yield 66%, white solid. M.p.: 207.2-209.3 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 7.1$  Hz, 2H), 7.65 (d,  $J = 7.6$  Hz, 2H), 7.46 (t,  $J = 7.5$  Hz, 2H), 7.40 – 7.31 (m, 3H), 7.30 – 7.21 (m, 4H), 7.06 (t,  $J = 7.7$  Hz, 4H), 6.73 – 6.63 (m, 3H), 6.25 (d,  $J = 2.1$  Hz, 1H), 6.13 (d,  $J = 2.2$  Hz, 1H), 6.03 – 5.88 (m, 1H), 5.35 (d,  $J = 17.3$ , 1H), 5.31 – 5.25 (m, 1H), 4.93 – 4.78 (m, 2H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.5, 143.3, 143.2, 141.1, 138.5, 133.5, 131.5, 129.8, 128.9, 128.6, 128.31, 128.29, 128.08, 128.05, 127.9, 127.5, 127.4, 127.0, 119.4, 117.3, 115.5, 81.4, 71.3, 66.5. HRMS calcd for  $\text{C}_{32}\text{H}_{27}\text{NO}_2$   $[\text{M}+\text{Na}]^+$ : 480.1934; Found: 480.1948.

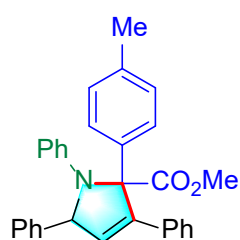


**Benzyl 1,2,3,5-tetraphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3e):** 200 mg, yield 79%, white solid. M.p.: 186.5-187.7 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 (d,  $J = 8.3$  Hz, 2H), 7.56 (d,  $J = 7.4$  Hz, 2H), 7.31 (d,  $J = 7.6$  Hz, 3H), 7.29 – 7.27 (m, 1H), 7.26 – 7.19 (m, 8H), 7.13 (t,  $J = 7.5$  Hz, 2H), 6.98 (t,  $J = 7.8$  Hz, 2H), 6.91 (d,  $J = 7.7$  Hz, 2H), 6.58 (t,  $J = 6.7$  Hz, 3H), 6.15 (d,  $J = 2.2$  Hz, 1H), 6.00 (d,  $J = 2.2$  Hz, 1H), 5.37 (d,  $J = 12.0$  Hz, 1H), 5.27 (d,  $J = 12.1$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.8, 143.2, 141.1, 138.6, 135.1, 133.5, 130.0, 129.0, 128.8, 128.60, 128.59, 128.5, 128.33, 128.32, 128.1, 128.0, 127.6, 127.4, 127.0, 117.3, 115.6, 81.4, 71.3, 67.9. HRMS calcd for  $\text{C}_{36}\text{H}_{29}\text{NO}_2$   $[\text{M}+\text{Na}]^+$ : 530.2091; Found: 530.2104.

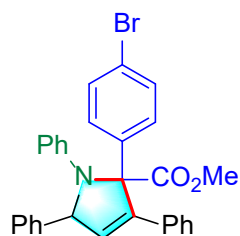


**Methyl 2-(4-methoxyphenyl)-1,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3f):** 186mg, yield 81%, white solid. M.p.: 236.2-238.7 °C.  $^1\text{H}$  NMR (400

MHz, CDCl<sub>3</sub>)  $\delta$  7.62 (d,  $J$  = 7.1 Hz, 2H), 7.44 (d,  $J$  = 9.0 Hz, 2H), 7.38 (t,  $J$  = 7.5 Hz, 2H), 7.29 (t,  $J$  = 7.3 Hz, 1H), 7.22 – 7.14 (m, 3H), 7.01 – 6.94 (m, 4H), 6.76 (d,  $J$  = 9.0 Hz, 2H), 6.58 (t,  $J$  = 7.3 Hz, 1H), 6.54 (d,  $J$  = 8.0 Hz, 2H), 6.15 (d,  $J$  = 2.2 Hz, 1H), 5.99 (d,  $J$  = 2.2 Hz, 1H), 3.84 (s, 3H), 3.75 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  171.7, 158.7, 143.4, 143.2, 141.2, 133.5, 130.4, 129.8, 129.3, 129.0, 128.4, 128.2, 128.1, 128.0, 127.4, 126.9, 117.1, 115.4, 113.4, 80.8, 71.1, 55.2, 52.6. HRMS calcd for C<sub>31</sub>H<sub>27</sub>NO<sub>3</sub> [M+Na]<sup>+</sup>: 484.1883; Found: 484.1879.

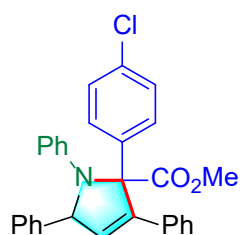


**Methyl 1,3,5-triphenyl-2-(p-tolyl)-2,5-dihydro-1H-pyrrole-2-carboxylate (3g):** 137mg, yield 62%, white solid. M.p.: 270.9-271.4 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.75 (d,  $J$  = 7.6 Hz, 2H), 7.55 (d,  $J$  = 8.0 Hz, 2H), 7.49 (t,  $J$  = 7.5 Hz, 2H), 7.38 (t,  $J$  = 7.4 Hz, 1H), 7.27 (q,  $J$  = 8.5 Hz, 3H), 7.14 (d,  $J$  = 8.1 Hz, 2H), 7.11 (d,  $J$  = 8.4 Hz, 3H), 7.07 (d,  $J$  = 8.0 Hz, 1H), 6.69 (d,  $J$  = 9.1 Hz, 3H), 6.26 (d,  $J$  = 2.2 Hz, 1H), 6.12 (d,  $J$  = 2.3 Hz, 1H), 3.92 (s, 3H), 2.35 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  171.5, 143.3, 143.2, 141.2, 137.1, 135.3, 133.4, 129.4, 128.9, 128.8, 128.4, 128.3, 128.1, 128.0, 127.9, 127.4, 126.8, 117.1, 115.4, 81.0, 77.5, 52.4, 21.1. HRMS calcd for C<sub>31</sub>H<sub>27</sub>NO<sub>2</sub> [M+Na]<sup>+</sup>: 468.1934; Found: 468.1950.

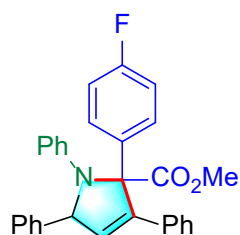


**Methyl 2-(4-bromophenyl)-1,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3h):** 188mg, yield 74%, yellow solid. M.p.: 230.1-230.8 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.64 (d,  $J$  = 7.3 Hz, 2H), 7.46 – 7.39 (m, 4H), 7.38 – 7.29 (m, 3H), 7.28 –

7.17 (m, 3H), 7.07 – 6.94 (m, 4H), 6.64 (d,  $J = 7.3$  Hz, 1H), 6.54 (d,  $J = 8.2$  Hz, 2H), 6.19 (d,  $J = 2.1$  Hz, 1H), 6.03 (d,  $J = 1.8$  Hz, 1H), 3.89 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.4, 142.9, 142.9, 140.8, 137.6, 132.9, 131.2, 130.4, 129.8, 129.0, 128.6, 128.4, 128.2, 128.1, 127.5, 126.9, 121.7, 117.5, 115.3, 80.6, 71.2, 52.8. HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{BrNO}_2$   $[\text{M}+\text{Na}]^+$ : 532.0883; Found: 532.0886.

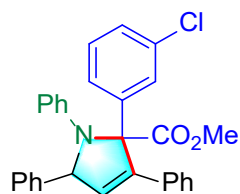


**Methyl 2-(4-chlorophenyl)-1,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3i)**: 111mg, yield 48%, white solid. M.p.: 232.8-234.0 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 7.6$  Hz, 2H), 7.57 (d,  $J = 8.4$  Hz, 2H), 7.48 (t,  $J = 7.5$  Hz, 2H), 7.38 (t,  $J = 7.3$  Hz, 1H), 7.29 (d,  $J = 8.3$  Hz, 5H), 7.13 – 7.04 (m, 4H), 6.70 (t,  $J = 7.3$  Hz, 1H), 6.63 (d,  $J = 8.2$  Hz, 2H), 6.26 (d,  $J = 2.1$  Hz, 1H), 6.10 (d,  $J = 2.2$  Hz, 1H), 3.95 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.4, 143.0, 142.9, 140.8, 137.1, 133.3, 132.9, 130.0, 129.8, 129.0, 128.6, 128.3, 128.19, 128.15, 128.1, 127.5, 126.9, 117.6, 115.3, 80.6, 71.2, 52.7. HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{ClNO}_2$   $[\text{M}+\text{Na}]^+$ : 488.1388; Found: 488.1396.

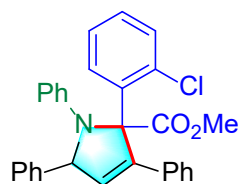


**Methyl 2-(4-fluorophenyl)-1,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3j)**: 81mg, yield 36%, white solid. M.p.: 266.8-267.4 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (d,  $J = 7.3$  Hz, 2H), 7.61 – 7.53 (m, 2H), 7.45 (t,  $J = 7.6$  Hz, 2H), 7.34 (t,  $J = 7.4$  Hz, 1H), 7.29 – 7.20 (m, 3H), 7.05 (t,  $J = 7.8$  Hz, 4H), 6.98 (d,  $J = 8.8$  Hz, 2H), 6.66 (t,  $J = 7.3$  Hz, 1H), 6.60 (d,  $J = 8.2$  Hz, 2H), 6.22 (d,  $J = 1.8$  Hz, 1H), 6.07 (d,  $J = 2.2$  Hz, 1H), 3.91 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.6, 161.9 (d,  $J = 246.9$  Hz), 143.2, 143.0, 140.9, 134.19, 134.16, 133.1, 130.4 (d,  $J = 8.0$  Hz), 129.6, 129.0, 128.5,

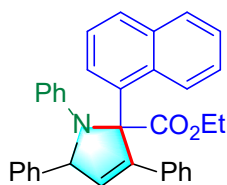
128.3, 128.1, 127.5, 126.9, 117.5, 115.4, 114.9 (d,  $J = 21.3$  Hz). 80.6, 71.2, 52.7.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -114.70 (s, 1F). HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{FNO}_2$   $[\text{M}+\text{Na}]^+$ : 472.1683; Found:472.1670.



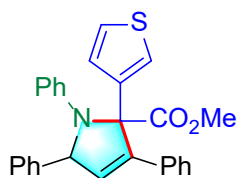
**Methyl 2-(3-chlorophenyl)-1,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3k)**: 139 mg, yield 60%, white solid. M.p.: 234.7-235.3 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 (d,  $J = 7.2$  Hz, 2H), 7.59 – 7.56 (m, 1H), 7.44 – 7.41 (m, 1H), 7.40 (t,  $J = 6.9$  Hz, 2H), 7.30 (t,  $J = 7.3$  Hz, 1H), 7.26 – 7.15 (m, 5H), 7.03 – 6.94 (m, 4H), 6.62 (t,  $J = 7.3$  Hz, 1H), 6.53 (d,  $J = 8.0$  Hz, 2H), 6.21 (d,  $J = 2.2$  Hz, 1H), 6.03 (d,  $J = 2.0$  Hz, 1H), 3.87 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.2, 142.9, 142.8, 140.8, 140.6, 134.0, 132.8, 130.1, 129.3, 129.0, 128.9, 128.6, 128.4, 128.2, 128.1, 127.8, 127.6, 126.9, 126.7, 117.6, 115.4, 80.6, 71.2, 52.8. HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{ClNO}_2$   $[\text{M}+\text{Na}]^+$ : 488.1388; Found: 488.1374.



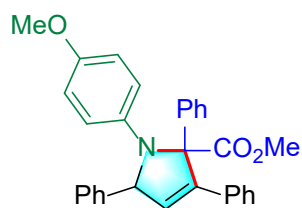
**Methyl 2-(2-chlorophenyl)-1,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3l)**: 102 mg, yield 44%, white solid. M.p.: 225.6-227.9 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (d,  $J = 7.5$  Hz, 1H), 7.48 (d,  $J = 7.3$  Hz, 2H), 7.39 (t,  $J = 7.5$  Hz, 2H), 7.35 – 7.25 (m, 4H), 7.24 – 7.10 (m, 3H), 7.01 – 6.92 (m, 2H), 6.90 (dd,  $J = 8.2, 1.5$  Hz, 2H), 6.70 – 6.61 (m, 3H), 6.30 (d,  $J = 2.5$  Hz, 1H), 5.94 (d,  $J = 2.3$  Hz, 1H), 3.85 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 143.0, 140.6, 137.8, 134.8, 133.4, 132.9, 132.4, 132.3, 132.2, 129.6, 128.9, 128.2, 127.9, 127.9, 127.6, 127.3, 126.8, 126.6, 117.5, 114.9, 82.8, 71.3, 52.4. HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{ClNO}_2$   $[\text{M}+\text{Na}]^+$ : 488.1388; Found: 488.1392.



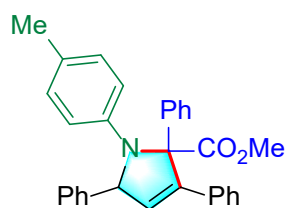
**Ethyl 2-(naphthalen-1-yl)-1,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3m):** 109 mg, yield 44%, white solid. M.p.: 233.3-234.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.99 (d, *J* = 9.4 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.81 (d, *J* = 9.4 Hz, 1H), 7.72 (d, *J* = 7.3 Hz, 1H), 7.62 (d, *J* = 7.5 Hz, 2H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.42 – 7.37 (m, 2H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 7.03 (t, *J* = 7.6 Hz, 2H), 6.84 (t, *J* = 7.8 Hz, 2H), 6.79 (d, *J* = 8.2 Hz, 2H), 6.70 (d, *J* = 7.7 Hz, 2H), 6.48 (t, *J* = 6.9 Hz, 1H), 6.42 (d, *J* = 2.5 Hz, 1H), 6.24 (d, *J* = 2.6 Hz, 1H), 4.45 – 4.31 (m, 2H), 1.18 (t, *J* = 7.1 Hz, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 171.8, 143.4, 142.4, 140.5, 135.5, 134.2, 132.6, 131.6, 130.3, 130.1, 129.4, 129.2, 129.0, 128.2, 127.7, 127.5, 127.4, 127.3, 126.8, 126.5, 125.8, 124.6, 123.5, 117.3, 115.2, 84.6, 70.3, 61.5, 13.9. HRMS calcd for C<sub>35</sub>H<sub>29</sub>NO<sub>2</sub> [M+Na]<sup>+</sup>: 518.2091; Found: 518.2102.



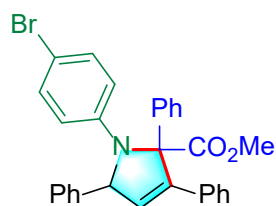
**Methyl 1,3,5-triphenyl-2-(thiophen-3-yl)-2,5-dihydro-1H-pyrrole-2-carboxylate (3n):** 168 mg, yield 77%, white solid. M.p.: 274.1-275.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.83 (dd, *J* = 3.0, 1.4 Hz, 1H), 7.66 (d, *J* = 7.0 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 1H), 7.24 – 7.17 (m, 3H), 7.10 (dd, *J* = 5.1, 3.0 Hz, 1H), 7.06 (dd, *J* = 8.0, 1.7 Hz, 2H), 6.99 (dd, *J* = 8.8, 7.2 Hz, 2H), 6.92 – 6.88 (m, 1H), 6.60 (t, *J* = 7.3 Hz, 1H), 6.52 (d, *J* = 7.8 Hz, 2H), 6.18 (d, *J* = 2.1 Hz, 1H), 5.94 (d, *J* = 2.1 Hz, 1H), 3.83 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 172.5, 143.2, 142.3, 141.1, 139.3, 132.9, 129.4, 129.0, 128.6, 128.3, 128.2, 127.8, 127.7, 127.5, 127.0, 125.3, 124.9, 117.5, 114.9, 78.6, 70.7, 52.9. HRMS calcd for C<sub>28</sub>H<sub>23</sub>NO<sub>2</sub>S [M+Na]<sup>+</sup>: 460.1342; Found: 460.1339.



**Methyl 1-(4-methoxyphenyl)-2,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3p):** 186 mg, yield 81%, white solid. M.p.: 203.4-204.7 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 (d,  $J = 8.1$  Hz, 2H), 7.49 (d,  $J = 8.6$  Hz, 2H), 7.39 (t,  $J = 7.6$  Hz, 2H), 7.29 (t,  $J = 7.3$  Hz, 1H), 7.25 – 7.20 (m, 3H), 7.20 – 7.14 (m, 3H), 6.99 (d,  $J = 8.0$  Hz, 2H), 6.59 – 6.54 (m, 2H), 6.54 – 6.49 (m, 2H), 6.19 (d,  $J = 2.2$  Hz, 1H), 5.97 (d,  $J = 2.2$  Hz, 1H), 3.86 (s, 3H), 3.62 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.8, 151.7, 143.3, 141.5, 138.5, 137.4, 133.5, 130.0, 128.9, 128.6, 128.2, 128.1, 128.04, 127.99, 127.5, 127.4, 127.0, 116.8, 114.0, 81.6, 71.4, 55.4, 52.5. HRMS calcd for  $\text{C}_{31}\text{H}_{27}\text{NO}_3$   $[\text{M}+\text{Na}]^+$ : 484.1883; Found: 484.1884.



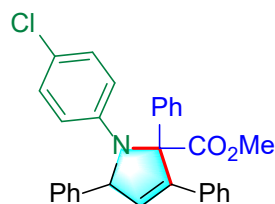
**Methyl 2,3,5-triphenyl-1-(p-tolyl)-2,5-dihydro-1H-pyrrole-2-carboxylate (3q):** 149 mg, yield 67%, white solid. M.p.: 226.7-229.1 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 7.5$  Hz, 2H), 7.65 (d,  $J = 7.6$  Hz, 2H), 7.49 (t,  $J = 7.6$  Hz, 2H), 7.39 (d,  $J = 7.3$  Hz, 1H), 7.34 (t,  $J = 7.7$  Hz, 2H), 7.28 (t,  $J = 7.7$  Hz, 4H), 7.09 (d,  $J = 8.6$  Hz, 2H), 6.89 (d,  $J = 8.1$  Hz, 2H), 6.60 (d,  $J = 8.2$  Hz, 2H), 6.27 (d,  $J = 2.3$  Hz, 1H), 6.12 (d,  $J = 2.3$  Hz, 1H), 3.94 (s, 3H), 2.21 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 143.3, 141.3, 140.9, 138.5, 133.4, 129.7, 129.0, 128.9, 128.5, 128.2, 128.1, 128.0, 127.9, 127.5, 127.4, 126.8, 126.2, 115.4, 81.2, 71.3, 52.4, 20.3. HRMS calcd for  $\text{C}_{31}\text{H}_{27}\text{NO}_2$   $[\text{M}+\text{Na}]^+$ : 468.1934; Found: 468.1950.





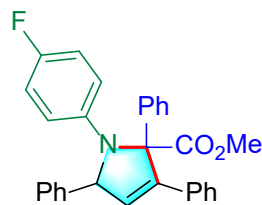
**Methyl 1-(4-bromophenyl)-2,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate**

**(3r)**: 186 mg, yield 73%, yellow solid. M.p.: 232.1-234.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 (d, *J* = 7.5 Hz, 2H), 7.55 (d, *J* = 6.9 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.36 (d, *J* = 7.3 Hz, 1H), 7.31 (t, *J* = 7.9 Hz, 2H), 7.28 – 7.23 (m, 2H), 7.20 (t, *J* = 7.2 Hz, 2H), 7.09 (d, *J* = 8.9 Hz, 2H), 6.99 (d, *J* = 8.9 Hz, 2H), 6.49 (d, *J* = 8.7 Hz, 2H), 6.20 (d, *J* = 2.2 Hz, 1H), 6.02 (d, *J* = 2.3 Hz, 1H), 3.89 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 171.0, 143.3, 142.2, 140.5, 137.9, 133.3, 131.1, 129.4, 129.1, 128.5, 128.24, 128.19, 128.18, 128.0, 127.8, 127.6, 126.7, 117.0, 109.7, 81.4, 71.4, 52.6. HRMS calcd for C<sub>30</sub>H<sub>24</sub>BrNO<sub>2</sub> [M+Na]<sup>+</sup>: 532.0883; Found: 532.0870.



**Methyl 1-(4-chlorophenyl)-2,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate**

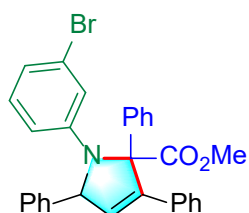
**(3s)**: 125 mg, yield 54%, white solid. M.p.: 231.5-233.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.58 (d, *J* = 7.3 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.9 Hz, 2H), 7.25 – 7.19 (m, 3H), 7.17 (d, *J* = 7.4 Hz, 2H), 6.95 – 6.87 (m, 4H), 6.46 (d, *J* = 9.0 Hz, 2H), 6.15 (d, *J* = 2.2 Hz, 1H), 5.97 (d, *J* = 2.3 Hz, 1H), 3.85 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 171.1, 143.3, 141.8, 140.6, 138.0, 133.3, 129.5, 129.1, 128.5, 128.29, 128.26, 128.23, 128.20, 128.0, 127.8, 127.7, 126.8, 122.3, 116.5, 81.5, 71.5, 52.7. HRMS calcd for C<sub>30</sub>H<sub>24</sub>ClNO<sub>2</sub> [M+Na]<sup>+</sup>: 488.1388; Found: 488.1402.



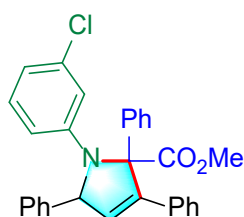
**Methyl 1-(4-fluorophenyl)-2,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate**

**(3t)**: 110 mg, yield 49%, white solid. M.p.: 257.6-258.9 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.60 (d, *J* = 7.0 Hz, 2H), 7.47 (d, *J* = 6.8 Hz, 2H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 7.27 – 7.19 (m, 4H), 7.16 (t, *J* = 7.2 Hz, 2H), 6.96 (d, *J* = 6.8 Hz, 2H),

6.67 (t,  $J = 8.8$  Hz, 2H), 6.52 – 6.44 (m, 2H), 6.18 (d,  $J = 2.2$  Hz, 1H), 5.96 (d,  $J = 2.2$  Hz, 1H), 3.86 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.4, 155.6 (d,  $J = 236.3$  Hz), 143.3, 140.9, 139.6, 139.5, 138.1, 133.4, 129.7, 129.0, 128.6, 128.17, 128.16, 128.0, 127.7 (d,  $J = 10.4$  Hz), 126.9, 116.4, 116.3, 114.9 (d,  $J = 22.0$  Hz), 81.6, 71.5, 52.6.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -126.20 (s, 1F). HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{FNO}_2$   $[\text{M}+\text{Na}]^+$ : 472.1683; Found: 472.1676.

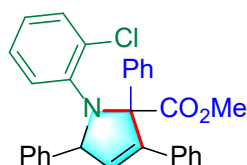


**Methyl 1-(3-bromophenyl)-2,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3u)**: 145 mg, yield 57%, yellow solid. M.p.: 188.3-189.3 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (d,  $J = 6.9$  Hz, 2H), 7.49 (d,  $J = 7.0$  Hz, 2H), 7.40 (t,  $J = 7.6$  Hz, 2H), 7.35 – 7.25 (m, 3H), 7.25 – 7.19 (m, 2H), 7.16 (t,  $J = 7.3$  Hz, 2H), 6.93 (d,  $J = 6.9$  Hz, 2H), 6.78 (t,  $J = 8.0$  Hz, 1H), 6.68 (d,  $J = 7.8$  Hz, 2H),  $\delta$  6.46 (d,  $J = 8.2$  Hz, 1H), 6.16 (d,  $J = 2.2$  Hz, 1H), 5.96 (d,  $J = 2.1$  Hz, 1H), 3.85 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.9, 144.5, 143.2, 140.4, 137.9, 133.3, 129.5, 129.5, 129.1, 128.5, 128.3, 128.24, 128.21, 128.0, 127.9, 127.8, 126.9, 122.4, 120.2, 118.3, 114.2, 81.5, 71.3, 52.7. HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{BrNO}_2$   $[\text{M}+\text{Na}]^+$ : 532.0883; Found: 532.0875.

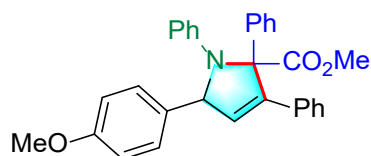


**Methyl 1-(3-chlorophenyl)-2,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3v)**: 126 mg, yield 54%, white solid. M.p.: 189.3-191.2 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 7.0$  Hz, 2H), 7.51 (d,  $J = 7.0$  Hz, 2H), 7.41 (t,  $J = 7.6$  Hz, 2H), 7.35 – 7.21 (m, 5H), 7.19 – 7.13 (m, 2H), 6.95 (d,  $J = 8.2$  Hz, 2H), 6.85 (t,  $J = 8.4$  Hz, 1H), 6.59 – 6.52 (m, 2H), 6.43 (d,  $J = 7.7$  Hz, 1H), 6.17 (d,  $J = 2.2$  Hz, 1H), 5.98 (d,  $J = 2.2$  Hz,

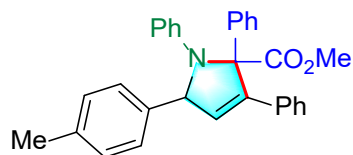
1H), 3.86 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.9, 144.4, 143.2, 140.5, 137.9, 134.1, 133.3, 129.5, 129.2, 129.1, 128.5, 128.3, 128.23, 128.21, 128.0, 127.9, 127.7, 126.8, 117.4, 115.4, 113.8, 81.6, 71.3, 52.7. HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{ClNO}_2$   $[\text{M}+\text{Na}]^+$ : 488.1388; Found: 488.1386.



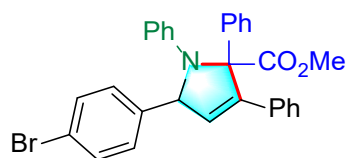
**Methyl 1-(2-chlorophenyl)-2,3,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3w):** 93 mg, yield 40%, white solid. M.p.: 205.4-207.2 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 (d,  $J = 7.8$  Hz, 1H), 7.52 (d,  $J = 7.0$  Hz, 2H), 7.42 (t,  $J = 7.6$  Hz, 2H), 7.35 – 7.27 (m, 4H), 7.21 – 7.14 (m, 3H), 7.03 – 6.98 (m, 2H), 6.95 (d,  $J = 8.4$  Hz, 2H), 6.71 (d,  $J = 8.1$  Hz, 2H), 6.68 (t,  $J = 7.3$  Hz, 1H), 6.34 (d,  $J = 2.5$  Hz, 1H), 5.99 (d,  $J = 2.5$  Hz, 1H), 3.87 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.7, 143.0, 140.5, 137.7, 134.8, 133.4, 132.8, 132.4, 132.3, 132.1, 129.6, 128.9, 128.1, 127.89, 127.85, 127.6, 127.3, 126.7, 126.6, 117.5, 114.9, 82.7, 71.2, 52.4. HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{ClNO}_2$   $[\text{M}+\text{Na}]^+$ : 488.1388; Found: 488.1387.



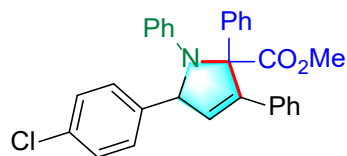
**Methyl 5-(4-methoxyphenyl)-1,2,3-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3x):** 154 mg, yield 67%, white solid. M.p.: 284.6-286.4 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.55 (d,  $J = 8.4$  Hz, 2H), 7.50 (d,  $J = 8.3$  Hz, 2H), 7.27 – 7.12 (m, 6H), 6.97 (t,  $J = 7.8$  Hz, 4H), 6.92 (d,  $J = 8.1$  Hz, 2H), 6.61 – 6.51 (m, 3H), 6.14 (d,  $J = 2.2$  Hz, 1H), 5.97 (d,  $J = 2.2$  Hz, 1H), 3.85 (s, 3H), 3.81 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.6, 159.0, 143.2, 143.0, 138.5, 133.5, 133.2, 129.9, 128.6, 128.4, 128.2, 128.11, 128.07, 128.0, 127.5, 117.2, 115.5, 114.4, 81.2, 70.7, 55.4, 52.6. HRMS calcd for  $\text{C}_{31}\text{H}_{27}\text{NO}_3$   $[\text{M}+\text{Na}]^+$ : 484.1883; Found: 484.1882



**Methyl 1,2,3-triphenyl-5-(p-tolyl)-2,5-dihydro-1H-pyrrole-2-carboxylate (3y):** 155 mg, yield 70%, white solid. M.p.: 276.3-278.2 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.54 (d,  $J = 7.8$  Hz, 4H), 7.30 – 7.15 (m, 8H), 6.99 (t,  $J = 7.9$  Hz, 4H), 6.61 (d,  $J = 7.3$  Hz, 1H), 6.58 (d,  $J = 8.3$  Hz, 2H), 6.17 (d,  $J = 2.2$  Hz, 1H), 6.02 (d,  $J = 2.2$  Hz, 1H), 3.87 (s, 3H), 2.39 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 143.2, 143.1, 138.4, 138.1, 137.0, 133.4, 129.8, 129.7, 128.6, 128.3, 128.2, 128.08, 128.06, 128.0, 127.5, 126.8, 117.2, 115.4, 81.2, 71.0, 52.5, 21.3. HRMS calcd for  $\text{C}_{31}\text{H}_{27}\text{NO}_2$   $[\text{M}+\text{Na}]^+$ : 468.1934; Found: 468.1941.

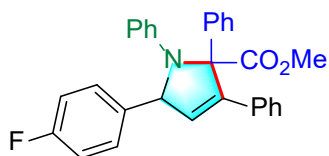


**Methyl 5-(4-bromophenyl)-1,2,3-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3z):** 183 mg, yield 72%, yellow solid. M.p.: 287.8-288.4 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 – 7.49 (m, 6H), 7.30 – 7.15 (m, 6H), 7.01 (d,  $J = 7.2$  Hz, 2H), 6.98 – 6.96 (m, 2H), 6.63 (t,  $J = 7.2$  Hz, 1H), 6.53 (d,  $J = 8.2$  Hz, 2H), 6.13 (d,  $J = 2.2$  Hz, 1H), 6.00 (d,  $J = 2.3$  Hz, 1H), 3.86 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.4, 143.8, 142.9, 140.3, 138.1, 133.2, 132.1, 129.0, 128.7, 128.54, 128.48, 128.3, 128.2, 128.1, 128.1, 127.7, 121.2, 117.6, 115.5, 81.4, 70.6, 52.6. HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{BrNO}_2$   $[\text{M}+\text{Na}]^+$ : 532.0883; Found: 532.0886.

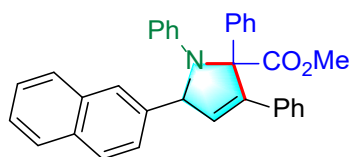


**Methyl 5-(4-chlorophenyl)-1,2,3-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3z1):** 160 mg, yield 69%, white solid. M.p.: 280.9-281.7 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (d,  $J = 8.5$  Hz, 2H), 7.47 (d,  $J = 8.1$  Hz, 2H), 7.35 (d,  $J = 8.5$  Hz, 2H), 7.24 – 7.13 (m, 6H), 6.99 – 6.96 (m, 2H), 6.93 (d,  $J = 7.0$  Hz, 2H), 6.59 (t,  $J = 7.3$  Hz,

1H), 6.49 (d,  $J = 7.9$  Hz, 2H), 6.10 (d,  $J = 2.2$  Hz, 1H), 5.98 (d,  $J = 2.2$  Hz, 1H), 3.84 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.4, 143.8, 142.9, 139.8, 138.2, 133.3, 133.2, 129.18, 129.15, 128.6, 128.5, 128.34, 128.30, 128.25, 128.13, 128.07, 127.7, 117.6, 115.5, 81.4, 70.6, 52.6. HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{ClNO}_2$   $[\text{M}+\text{Na}]^+$ : 488.1388; Found: 488.1394.

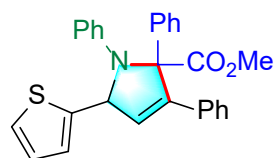


**Methyl 5-(4-fluorophenyl)-1,2,3-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3z2):** 153 mg, yield 68%, white solid. M.p.: 264.7-266.0 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 – 7.58 (m, 2H), 7.51 (d,  $J = 7.0$  Hz, 2H), 7.28 – 7.14 (m, 6H), 7.09 (t,  $J = 8.7$  Hz, 2H), 7.03 – 6.94 (m, 4H), 6.61 (t,  $J = 7.3$  Hz, 1H), 6.53 (d,  $J = 8.3$  Hz, 2H), 6.14 (d,  $J = 2.2$  Hz, 1H), 6.02 (d,  $J = 2.2$  Hz, 1H), 3.86 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 162.2 (d,  $J = 245.1$  Hz), 143.5, 143.0, 138.2, 136.9 (d,  $J = 2.9$  Hz), 133.3, 129.5, 128.54, 128.45, 128.4, 128.24, 128.20, 128.10, 128.05, 127.6, 117.5, 115.8 (d,  $J = 21.4$  Hz), 115.5, 81.3, 70.5, 52.7.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -129.66 (s, 1F). HRMS calcd for  $\text{C}_{30}\text{H}_{24}\text{FNO}_2$   $[\text{M}+\text{Na}]^+$ : 472.1683; Found: 472.1696.

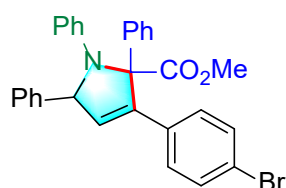


**Methyl 5-(naphthalen-2-yl)-1,2,3-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3z3):** 132 mg, yield 55%, yellow solid. M.p.: 303.7-304.8 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (s, 1H), 7.87 (t,  $J = 8.3$  Hz, 2H), 7.85 – 7.78 (m, 2H), 7.54 (d,  $J = 7.1$  Hz, 2H), 7.48 (t,  $J = 6.2$  Hz, 2H), 7.26 (t,  $J = 7.3$  Hz, 2H), 7.23 – 7.13 (m, 4H), 6.99 – 6.91 (m, 4H), 6.62 – 6.58 (m, 2H), 6.56 (d,  $J = 7.2$  Hz, 1H), 6.22 – 6.16 (m, 2H), 3.92 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 143.5, 143.2, 138.9, 138.4, 133.8, 133.4, 133.1, 129.5, 128.9, 128.6, 128.4, 128.3, 128.2, 128.13, 128.06, 128.0, 127.9, 127.6, 126.2, 125.9, 125.7, 125.0, 117.3, 115.5, 81.4, 71.5, 52.6. HRMS calcd for  $\text{C}_{34}\text{H}_{27}\text{NO}_2$   $[\text{M}$

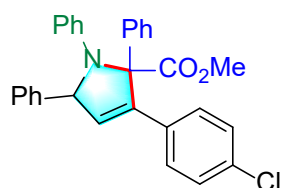
+Na]<sup>+</sup>: 504.1934; Found: 504.1947.



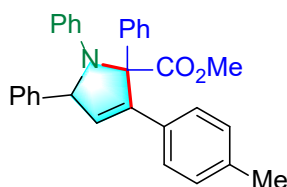
**Methyl 1,2,3-triphenyl-5-(thiophen-2-yl)-2,5-dihydro-1H-pyrrole-2-carboxylate (3z4):** 92 mg, yield 42%, white solid. M.p.: 279.0-280.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.48 (d, *J* = 7.0 Hz, 2H), 7.27 – 7.23 (m, 3H), 7.22 – 7.14 (m, 5H), 7.02 – 6.94 (m, 5H), 6.65 (d, *J* = 8.3 Hz, 2H), 6.60 (t, *J* = 7.2 Hz, 1H), 6.34 (d, *J* = 2.3 Hz, 1H), 6.18 (d, *J* = 2.2 Hz, 1H), 3.85 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 171.3, 146.1, 143.7, 142.9, 138.1, 133.2, 128.8, 128.6, 128.4, 128.29, 128.25, 128.1, 127.6, 126.8, 125.4, 125.2, 117.6, 115.3, 80.7, 66.4, 52.5. HRMS calcd for C<sub>28</sub>H<sub>23</sub>NO<sub>2</sub>S [M+Na]<sup>+</sup>: 460.1342; Found: 460.1347.



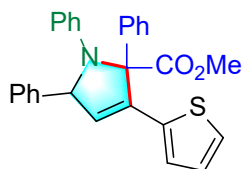
**Methyl 3-(4-bromophenyl)-1,2,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3z5):** 157 mg, yield 62%, yellow solid. M.p.: 269.5-270.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.66 (d, *J* = 7.9 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.38 – 7.30 (m, 4H), 7.29 (d, *J* = 6.8 Hz, 1H), 7.25 – 7.21 (m, 1H), 7.01 (t, *J* = 7.3 Hz, 2H), 6.85 (d, *J* = 7.0 Hz, 2H), 6.66 – 6.56 (m, 3H), 6.22 (d, *J* = 3.4 Hz, 1H), 6.06 (d, *J* = 2.2 Hz, 1H), 3.88 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 171.1, 142.9, 142.1, 140.8, 138.2, 132.4, 131.1, 130.3, 129.8, 129.0, 128.4, 128.3, 128.2, 127.8, 127.5, 126.8, 122.3, 117.4, 115.5, 81.3, 71.1, 52.6. HRMS calcd for C<sub>30</sub>H<sub>24</sub>BrNO<sub>2</sub> [M+Na]<sup>+</sup>: 532.0883; Found: 532.0878.



**Methyl 3-(4-chlorophenyl)-1,2,5-triphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (3z6):** 137 mg, yield 59%, white solid. M.p.: 278.9-280.2 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.66 (d, *J* = 7.6 Hz, 2H), 7.55 (d, *J* = 7.9 Hz, 2H), 7.43 (t, *J* = 7.0 Hz, 2H), 7.37 – 7.27 (m, 3H), 7.26 – 7.22 (m, 1H), 7.17 (d, *J* = 8.5 Hz, 2H), 7.00 (t, *J* = 7.5 Hz, 2H), 6.92 (d, *J* = 7.0 Hz, 2H), 6.66 – 6.54 (m, 3H), 6.21 (d, *J* = 3.5 Hz, 1H), 6.07 (d, *J* = 2.2 Hz, 1H), 3.89 (s, 3H); <sup>13</sup>C {<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 171.1, 142.9, 142.1, 140.8, 138.2, 134.0, 131.9, 130.2, 129.5, 129.0, 128.4, 128.3, 128.23, 128.18, 127.8, 127.5, 126.8, 117.4, 115.5, 81.3, 71.1, 52.6. HRMS calcd for C<sub>30</sub>H<sub>24</sub>ClNO<sub>2</sub> [M+Na]<sup>+</sup>: 488.1388; Found: 488.1384.

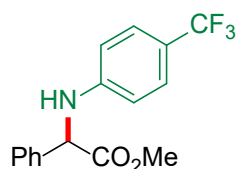


**Methyl 1,2,5-triphenyl-3-(p-tolyl)-2,5-dihydro-1H-pyrrole-2-carboxylate (3z7):** 155 mg, yield 70%, white solid. M.p.: 261.9-263.4 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.66 (d, *J* = 6.8 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.26 (t, *J* = 7.5 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.03 – 6.96 (m, 4H), 6.90 (d, *J* = 8.2 Hz, 2H), 6.61 (d, *J* = 7.3 Hz, 1H), 6.58 (d, *J* = 8.1 Hz, 2H), 6.16 (d, *J* = 2.2 Hz, 1H), 6.04 (d, *J* = 2.3 Hz, 1H), 3.88 (s, 3H), 2.30 (s, 3H); <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>) δ 171.5, 143.22, 143.20, 141.2, 138.5, 137.9, 130.4, 129.0, 128.9, 128.7, 128.6, 128.4, 128.04, 128.03, 127.5, 127.4, 126.9, 117.2, 115.4, 81.2, 71.2, 52.6, 21.3. HRMS calcd for C<sub>31</sub>H<sub>27</sub>NO<sub>2</sub> [M+Na]<sup>+</sup>: 468.1934; Found: 468.1942.

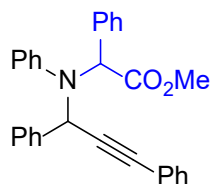


**Methyl 1,2,5-triphenyl-3-(thiophen-2-yl)-2,5-dihydro-1H-pyrrole-2-carboxylate (3z8):** 89 mg, yield 41%, white solid. M.p.: 227.1-229.0 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.68 – 7.60 (m, 4H), 7.47 – 7.38 (m, 2H), 7.37 – 7.25 (m, 3H), 7.25 – 7.19 (m, 1H),

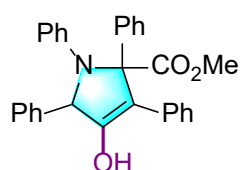
7.13 (d,  $J = 5.0$  Hz, 1H), 7.05 – 6.96 (m, 2H), 6.87 (t,  $J = 4.4$  Hz, 1H), 6.83 (d,  $J = 3.7$  Hz, 1H), 6.66 – 6.57 (m, 3H), 6.27 (d,  $J = 3.5$  Hz, 1H), 6.07 (d,  $J = 2.3$  Hz, 1H), 3.91 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.2, 143.0, 140.8, 138.2, 137.2, 135.2, 129.0, 128.8, 128.6, 128.4, 128.1, 127.7, 127.5, 127.1, 126.8, 126.5, 125.3, 117.3, 115.3, 80.8, 71.2, 52.7. HRMS calcd for  $\text{C}_{28}\text{H}_{23}\text{NO}_2\text{S}$   $[\text{M}+\text{Na}]^+$ : 460.1342; Found: 460.1347.



**Methyl-2-phenyl-2-((4-(trifluoromethyl)phenyl)amino)acetate (3z9')**: 34 mg, yield 22%, white solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.49 (dd,  $J = 8.3$  Hz, 2H), 7.41 – 7.31 (m, 5H), 6.57 (d,  $J = 8.3$  Hz, 2H), 5.38 (s, 1H), 5.11 (s, 1H), 3.76 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.9, 148.4, 136.9, 129.2, 128.7, 127.3,  $\delta$  126.7 (q,  $J = 3.8$  Hz), 124.9 (q,  $J = 272.3$  Hz), 119.8 (q,  $J = 32.5$  Hz), 112.8, 60.3, 53.1.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -61.16 (s, 3F).



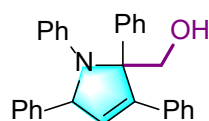
**Methyl 2-((1,3-diphenylprop-2-yn-1-yl)(phenyl)amino)-2-phenylacetate (4b)**: 42 mg, yield 10%, white solid. M.p.: 250.6-252.6 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 – 7.65 (m, 2H), 7.38 – 7.29 (m, 5H), 7.30 – 7.21 (m, 7H), 7.16 (d,  $J = 8.4$  Hz, 2H), 6.98 (t,  $J = 7.7$  Hz, 2H), 6.64 (t,  $J = 7.3$  Hz, 1H), 6.50 (d,  $J = 8.0$  Hz, 2H), 4.96 (s, 1H), 3.64 (s, 3H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  172.4, 145.0, 136.6, 136.3, 131.7, 129.9, 129.0, 128.6, 128.3, 128.3, 128.2, 128.1, 128.0, 127.9, 123.2, 118.0, 116.0, 88.5, 86.3, 70.8, 52.9, 48.4. HRMS calcd for  $\text{C}_{30}\text{H}_{25}\text{NO}_2$   $[\text{M}+\text{Na}]^+$ : 454.1778; Found: 454.1788.





**Methyl 4-hydroxy-1,2,3,5-tetraphenyl-2,5-dihydro-1H-pyrrole-2-carboxylate (5):**

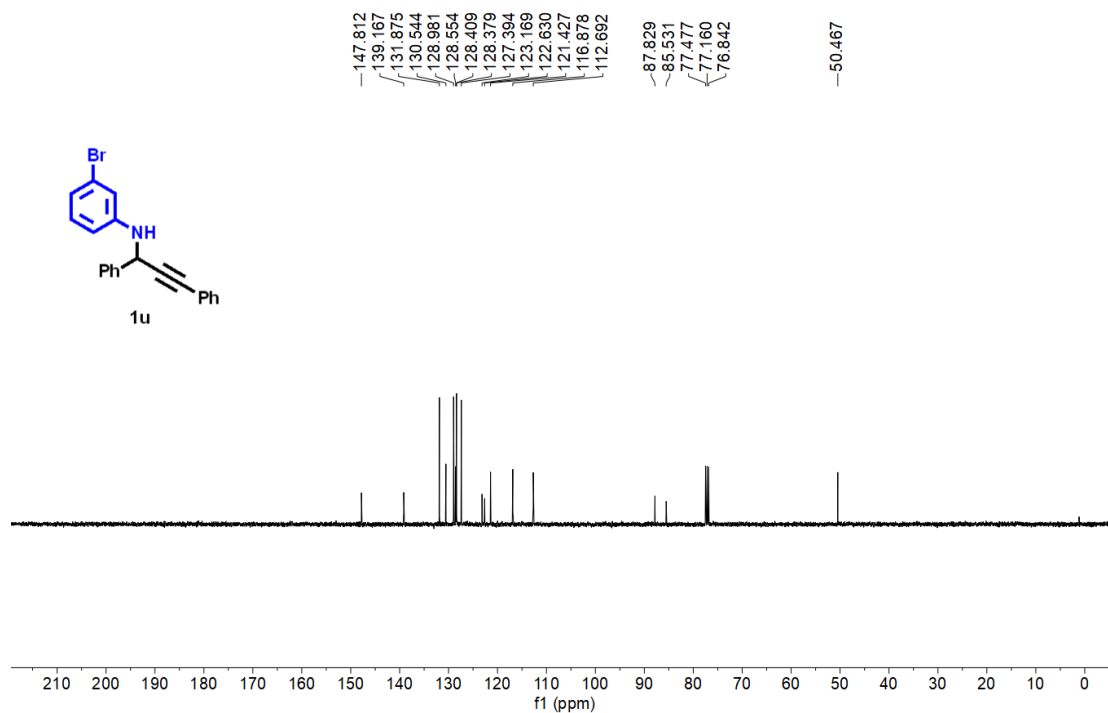
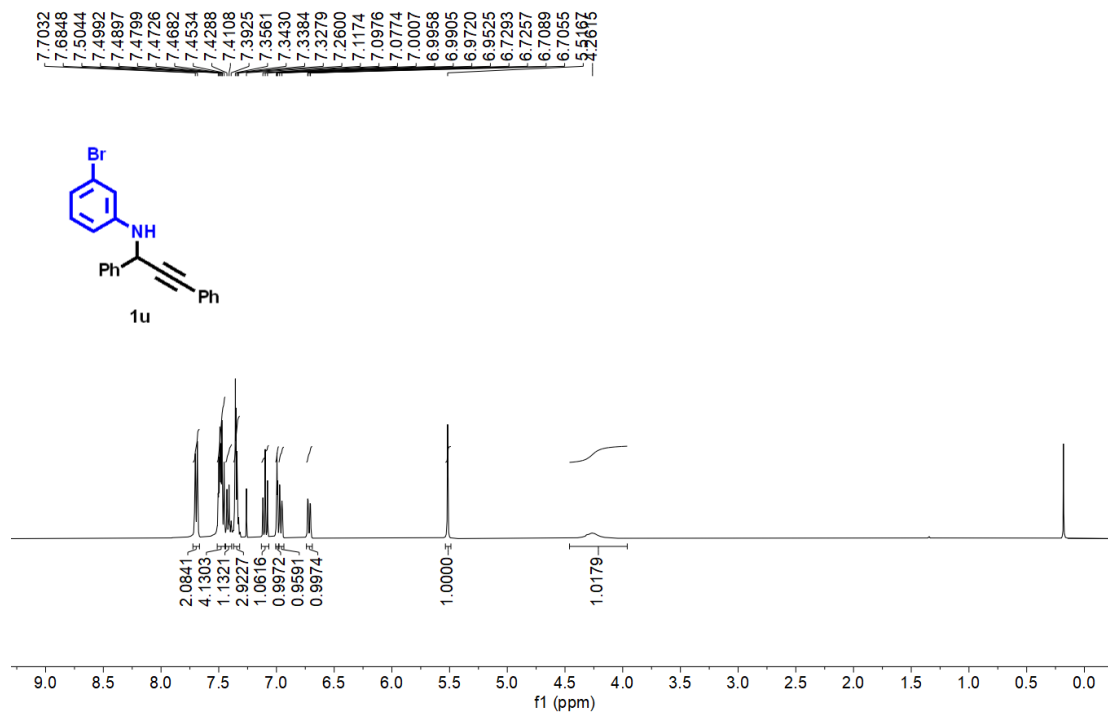
170 mg, yield 76%, white solid. M.p.: 231.6-232.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.57 (s, 1H), 7.43 – 7.36 (m, 4H), 7.35 – 7.27 (m, 5H), 7.27 – 7.20 (m, 6H), 6.86 (t, *J* = 7.7 Hz, 1H), 6.69 (d, *J* = 8.2 Hz, 1H), 6.54 (s, 1H), 6.32 (t, *J* = 7.5 Hz, 1H), 6.05 (d, *J* = 7.8 Hz, 1H), 5.33 (s, 1H), 3.57 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 175.2, 156.0, 141.3, 140.9, 137.1, 133.4, 133.2, 130.1, 128.6, 128.5, 128.3, 128.2, 128.12, 128.08, 128.01, 127.98, 127.7, 118.9, 115.2, 85.3, 75.4, 52.9. HRMS calcd for C<sub>30</sub>H<sub>25</sub>NO<sub>3</sub> [M+Na]<sup>+</sup>: 470.1727; Found: 470.1729.

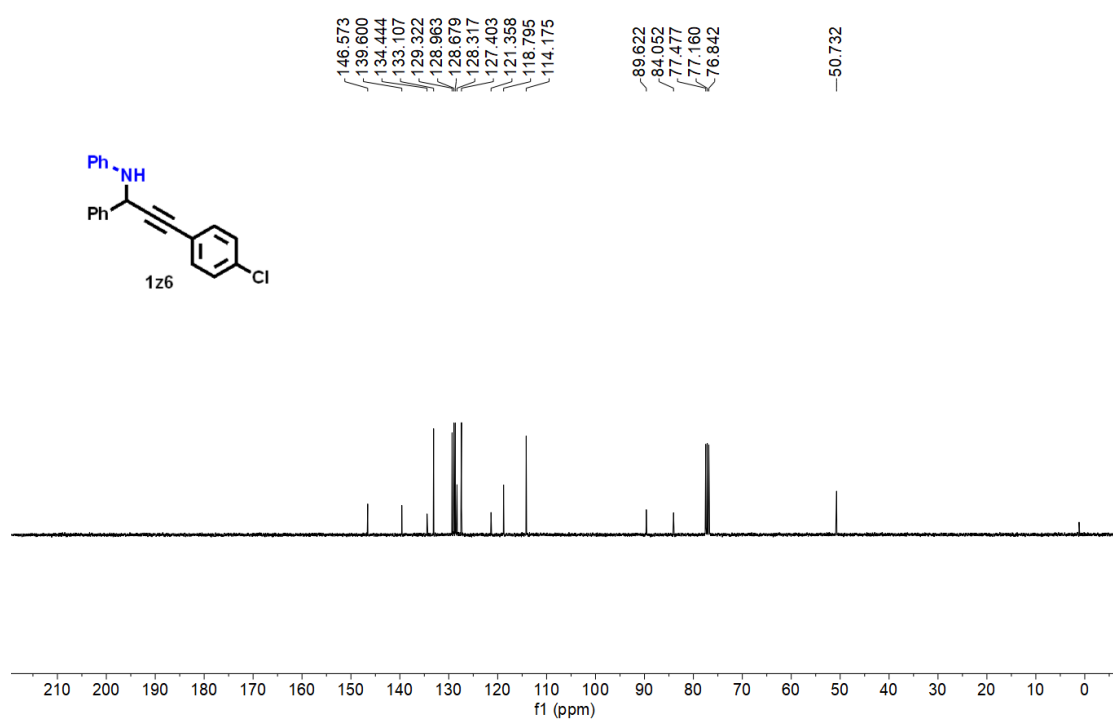
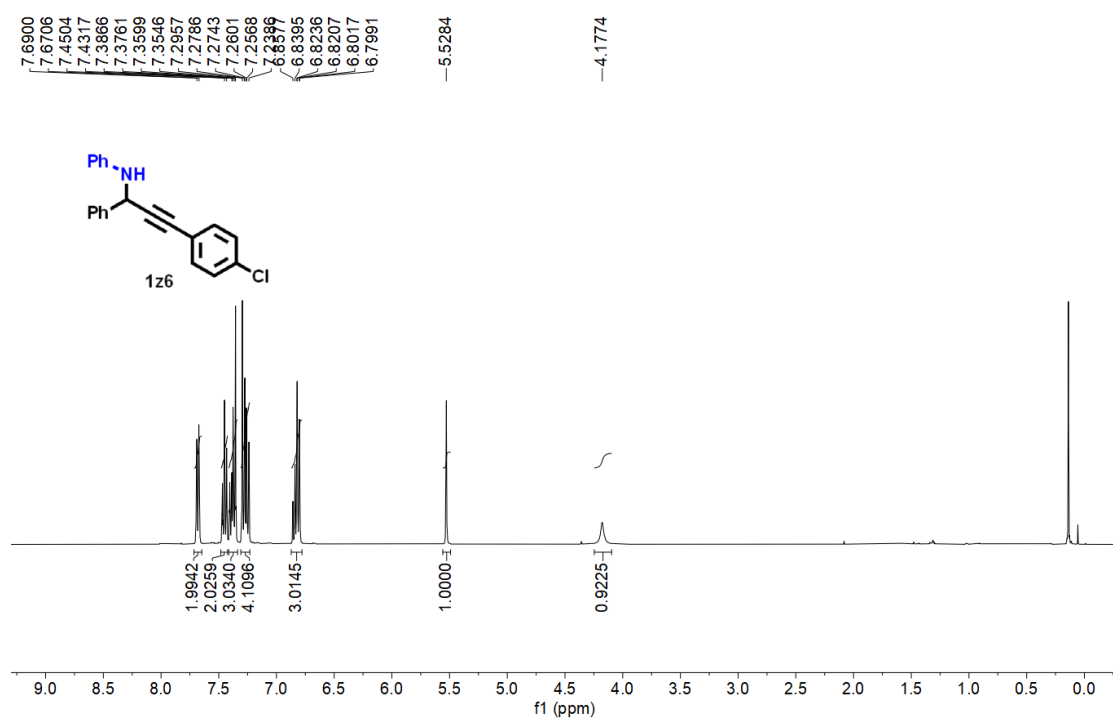


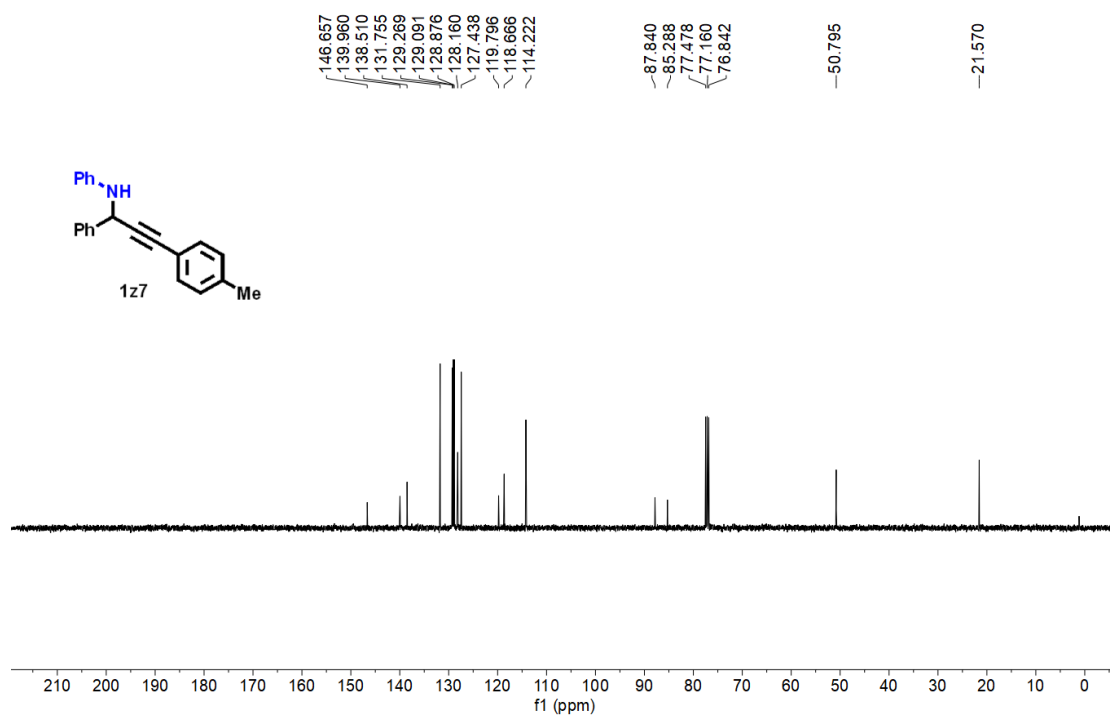
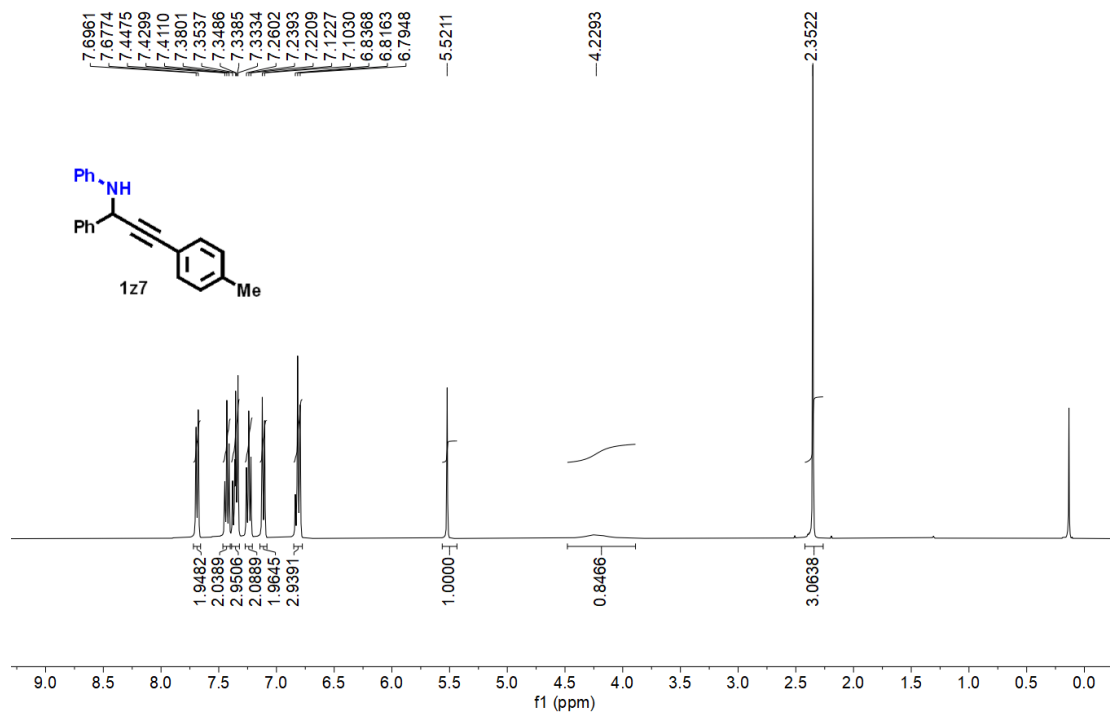
**(1,2,3,5-tetraphenyl-2,5-dihydro-1H-pyrrol-2-yl) Methanol (6):** 179 mg, yield 89%

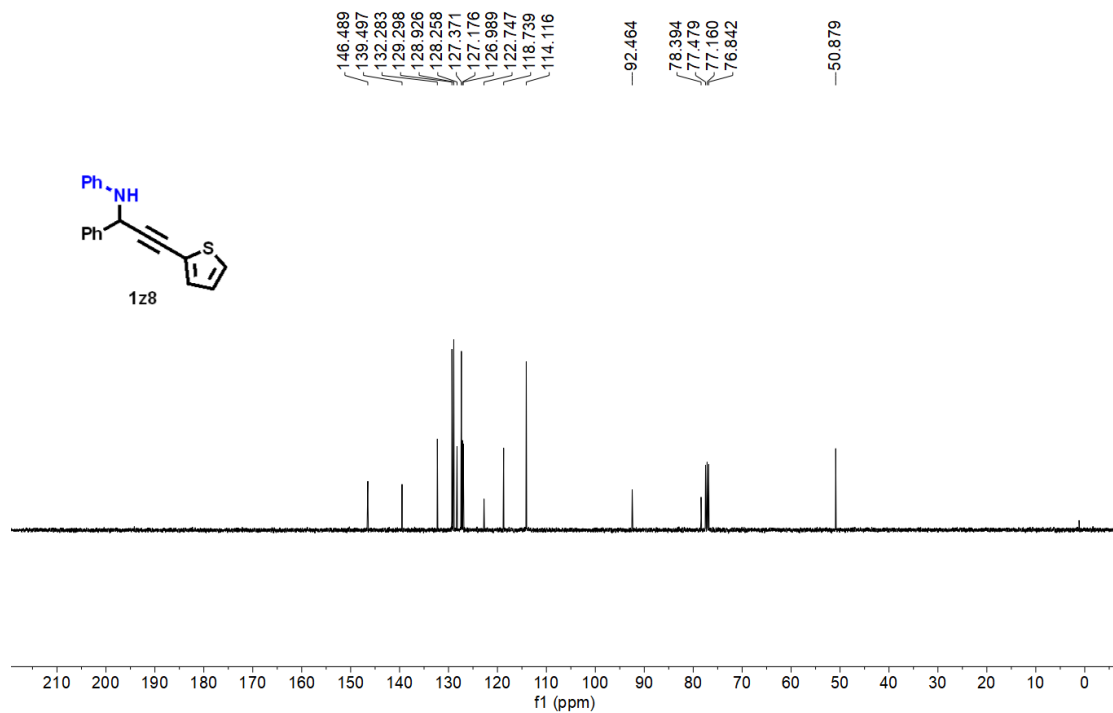
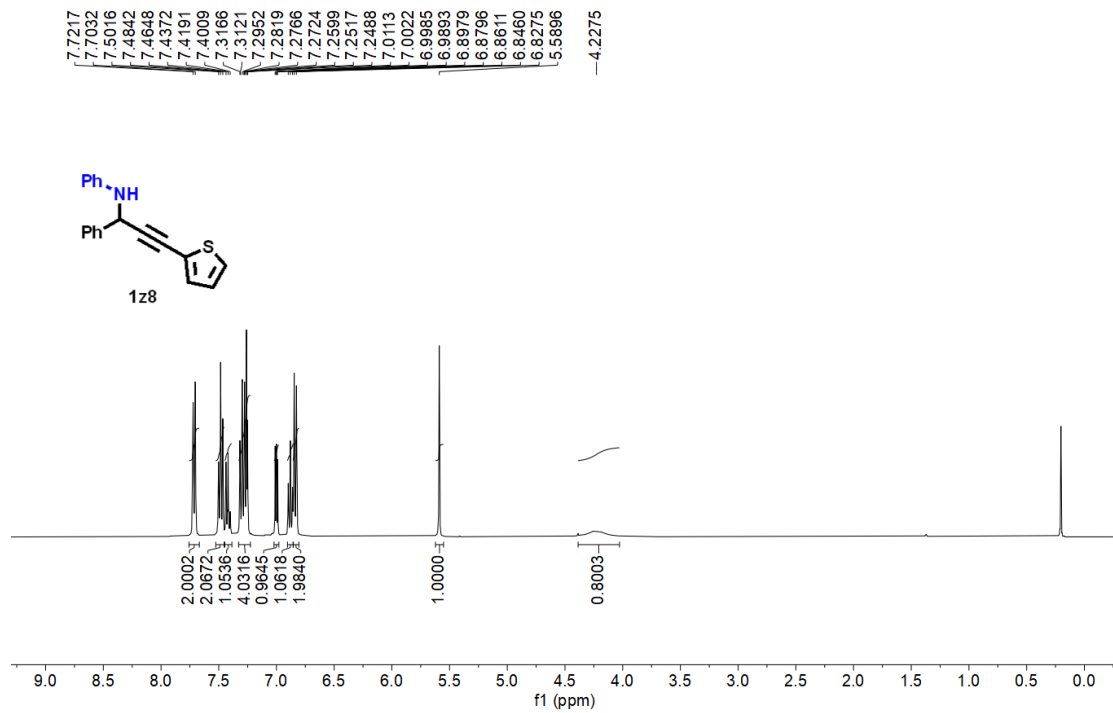
white solid. M.p.: 201.1-204.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 (d, *J* = 6.9 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.37 – 7.31 (m, 3H), 7.30 – 7.25 (m, 4H), 7.21 (t, *J* = 7.4 Hz, 2H), 7.04 – 7.00 (m, 2H), 6.94 (d, *J* = 7.0 Hz, 2H), 6.74 – 6.63 (m, 3H), 6.20 (d, *J* = 2.0 Hz, 1H), 6.03 (d, *J* = 2.1 Hz, 1H), 4.74 (d, *J* = 8.8 Hz, 1H), 4.42 – 4.31 (m, 1H), 2.48 (d, *J* = 9.0 Hz, 1H); <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) δ 145.0, 144.4, 141.8, 140.7, 134.4, 129.16, 129.15, 128.7, 128.5, 128.3, 128.2, 128.1, 127.7, 127.5, 127.3, 126.7, 118.9, 117.9, 80.4, 70.8, 62.6. HRMS calcd for C<sub>29</sub>H<sub>25</sub>NO [M+Na]<sup>+</sup>: 426.1828; Found: 426.1830.

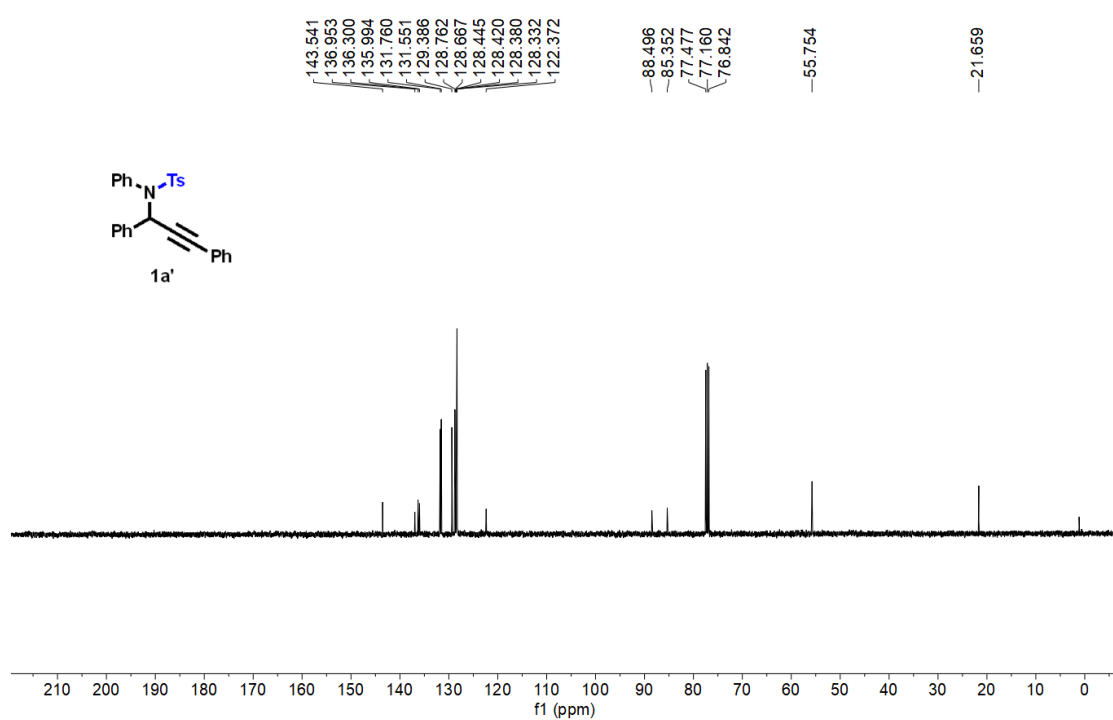
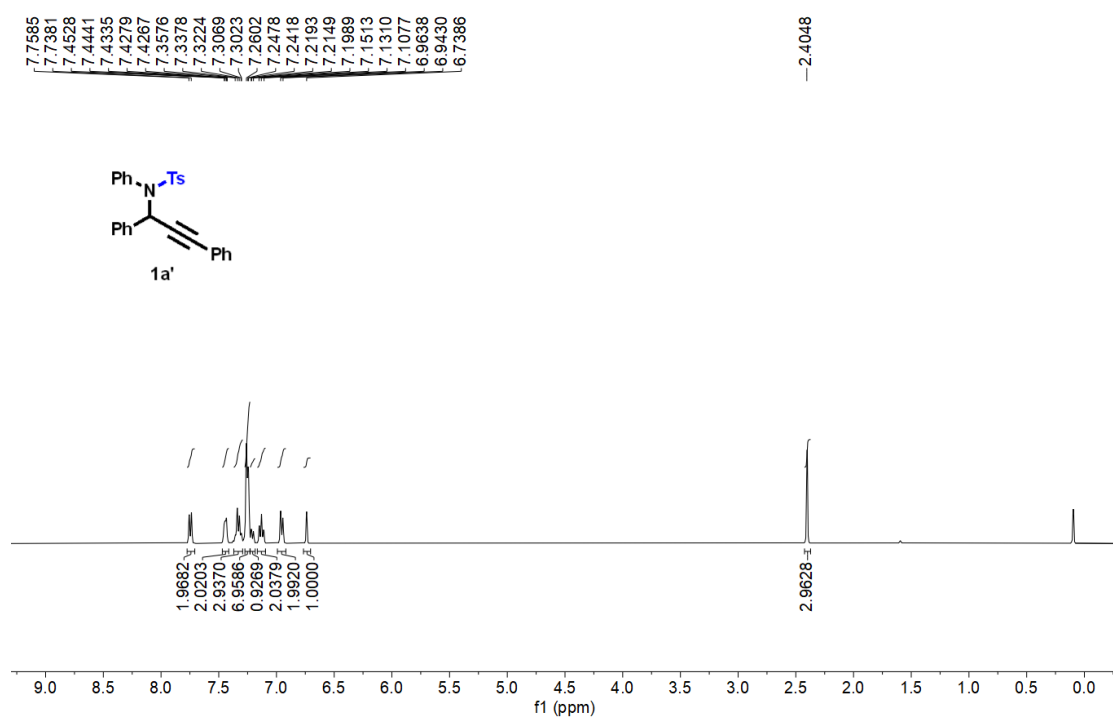
## 9. Copies of NMR spectra for compounds

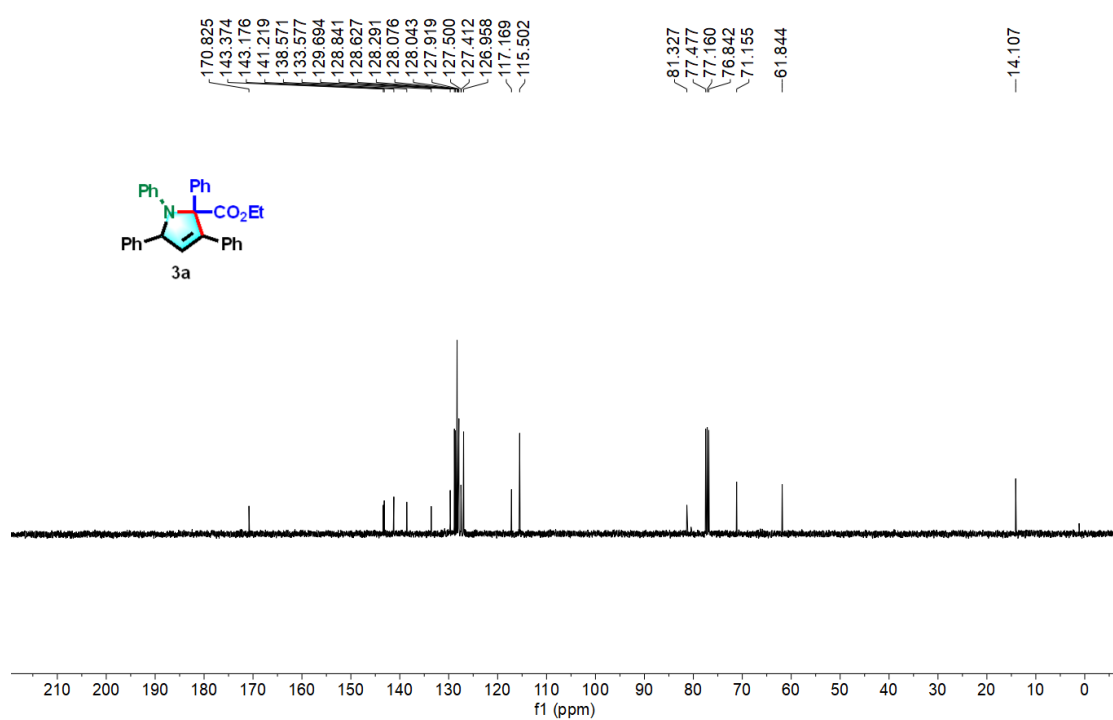
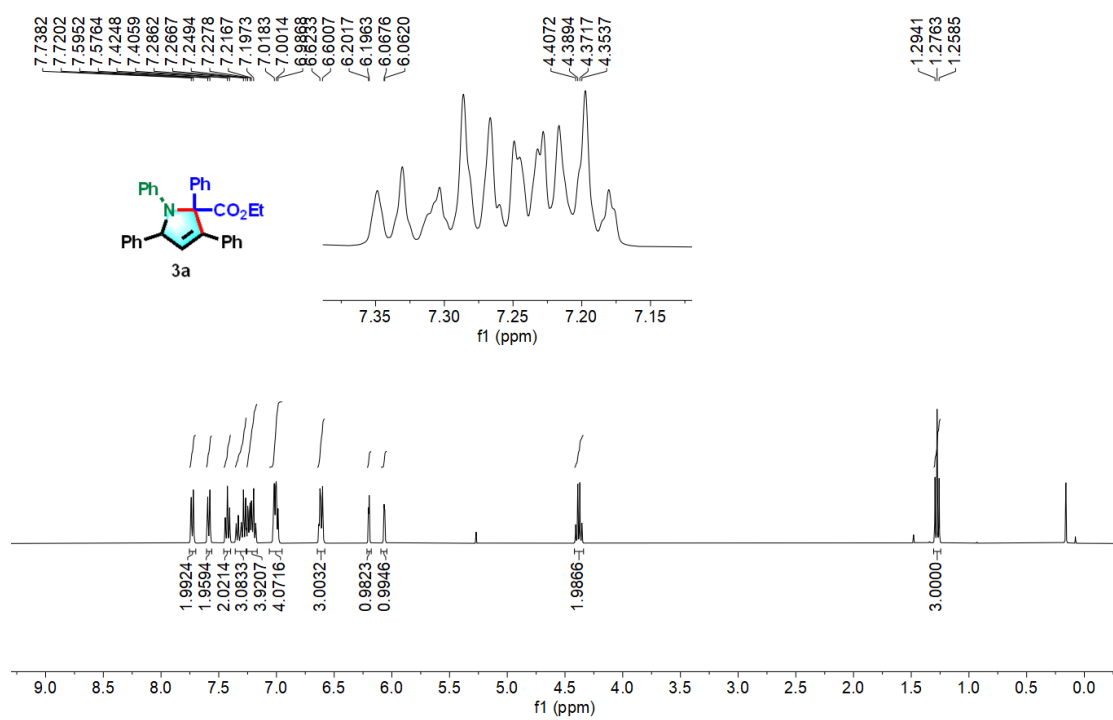


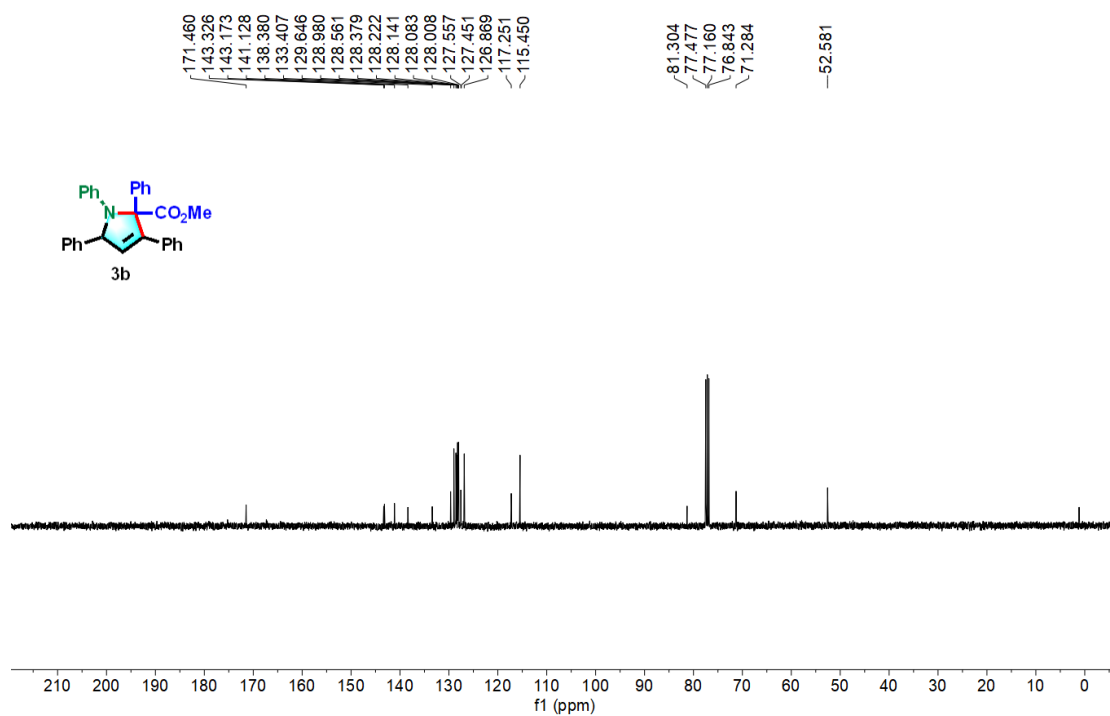
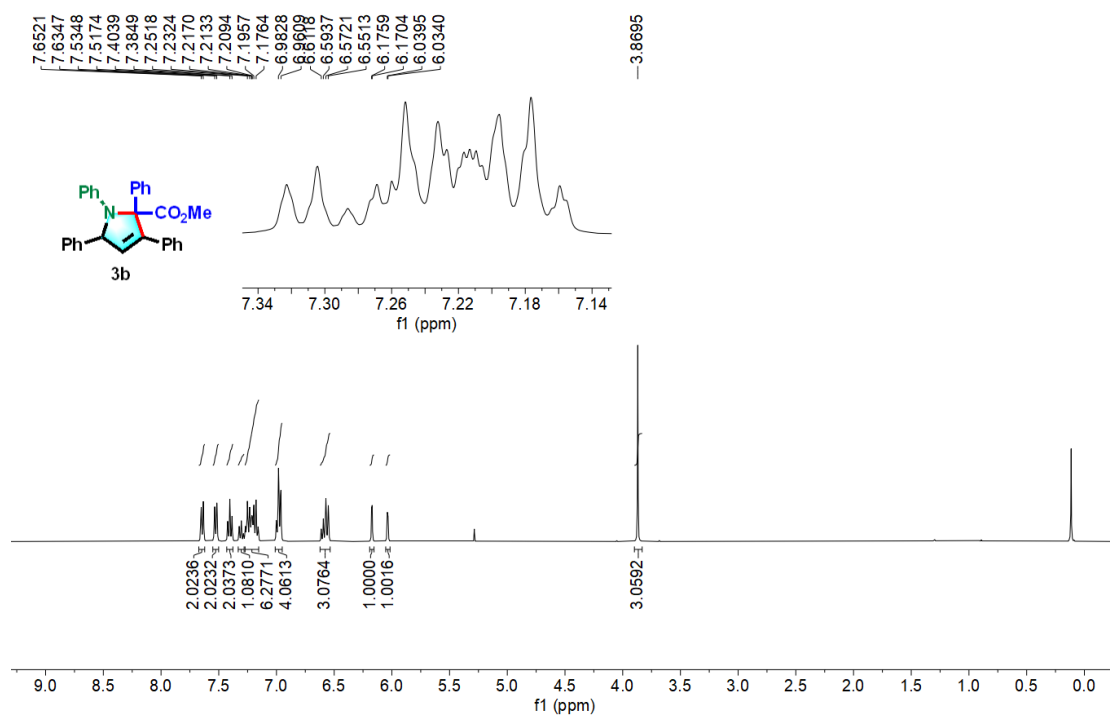




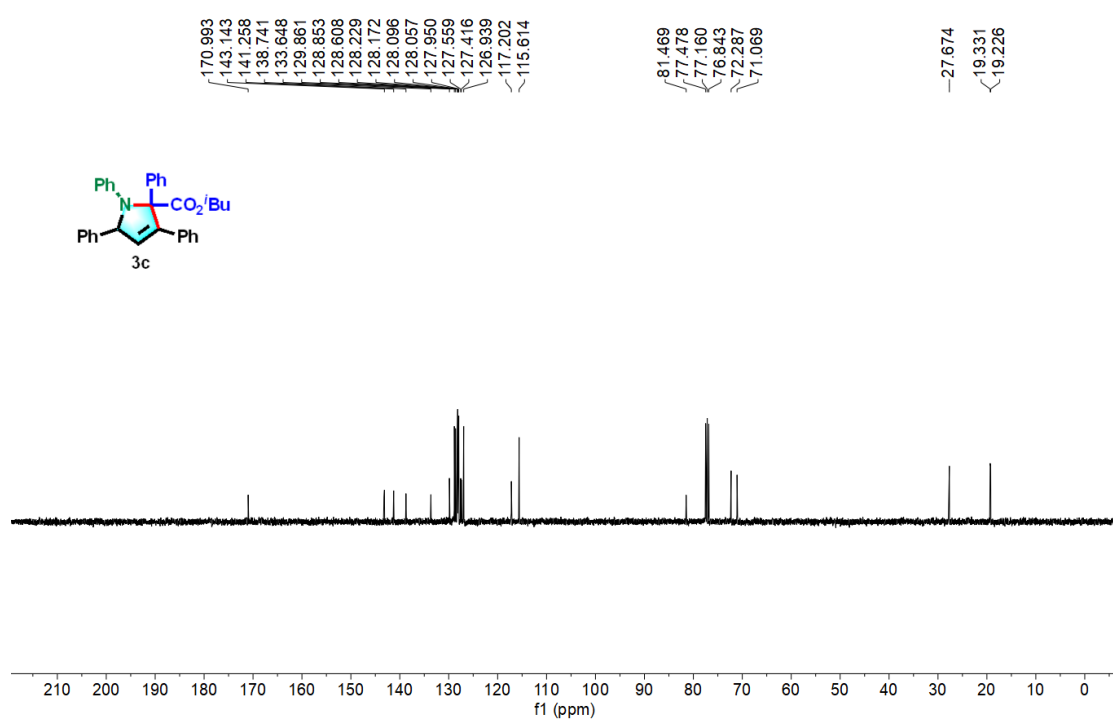
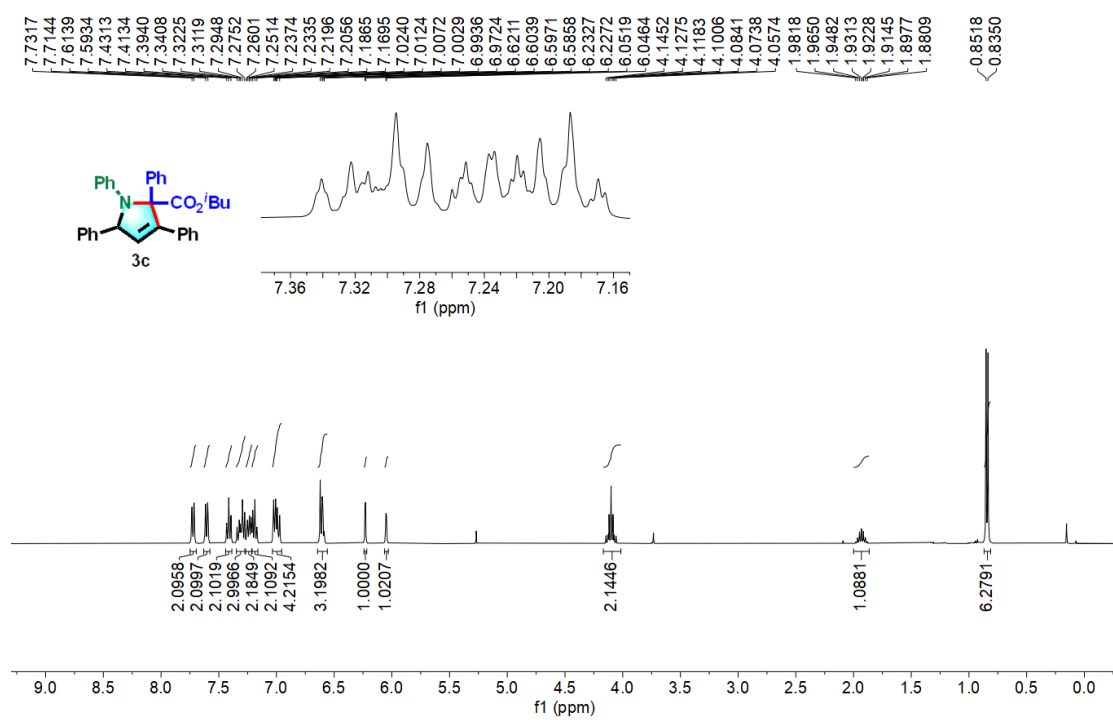


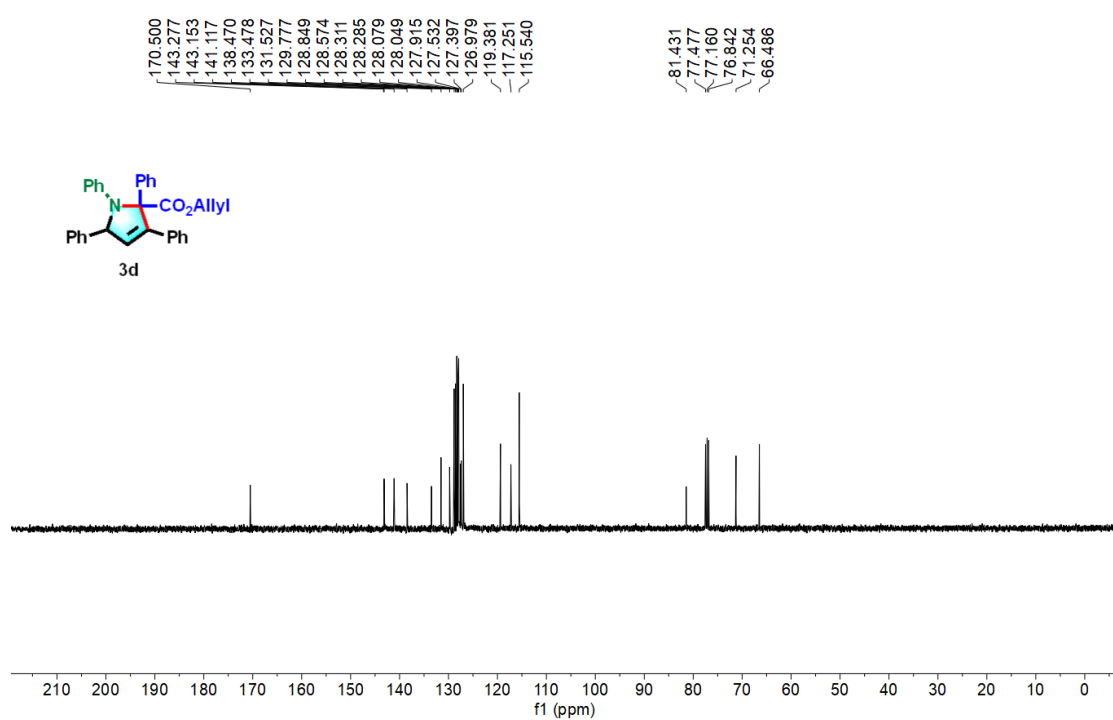
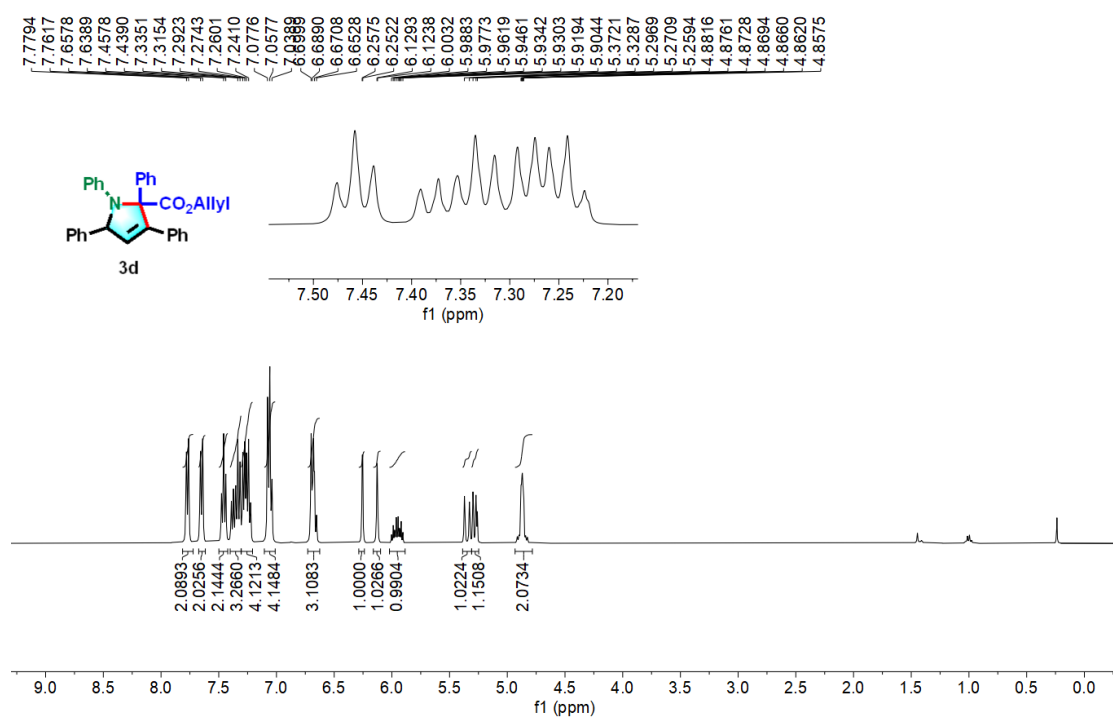


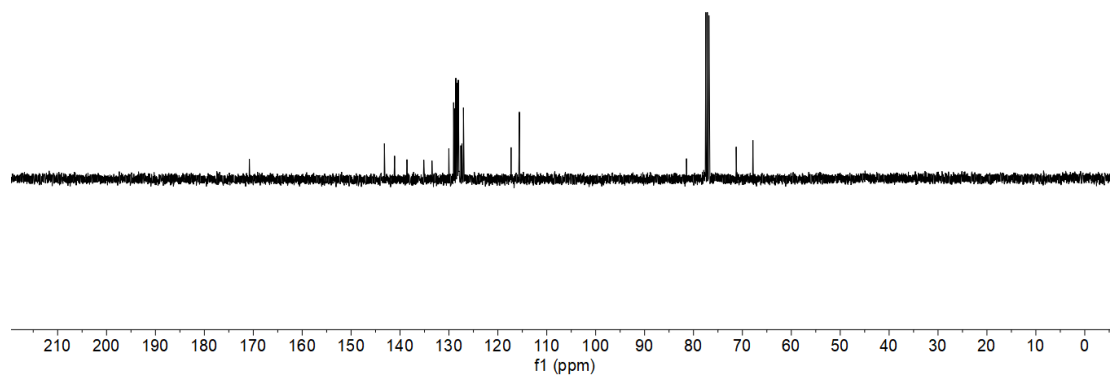
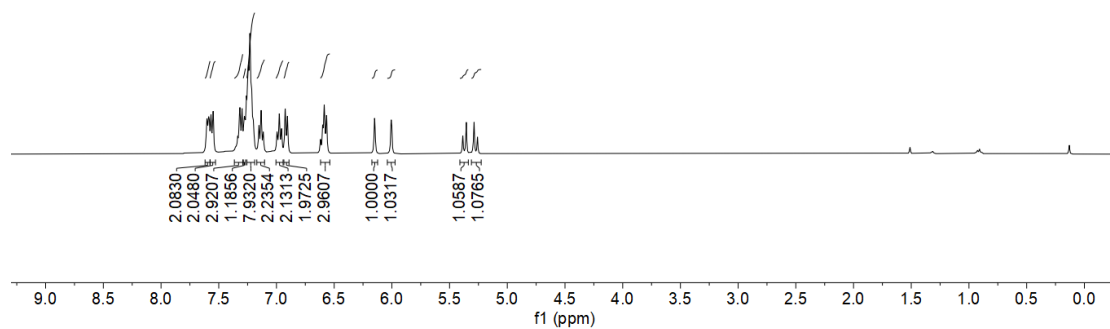
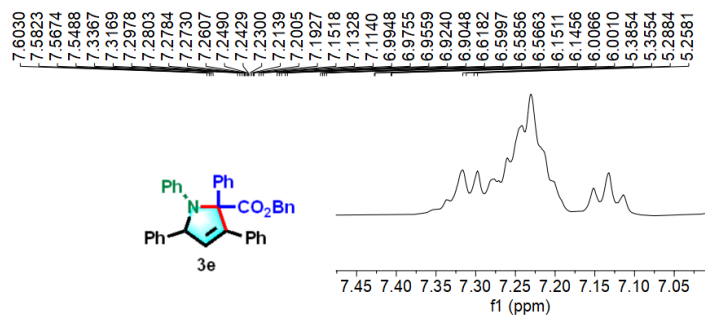


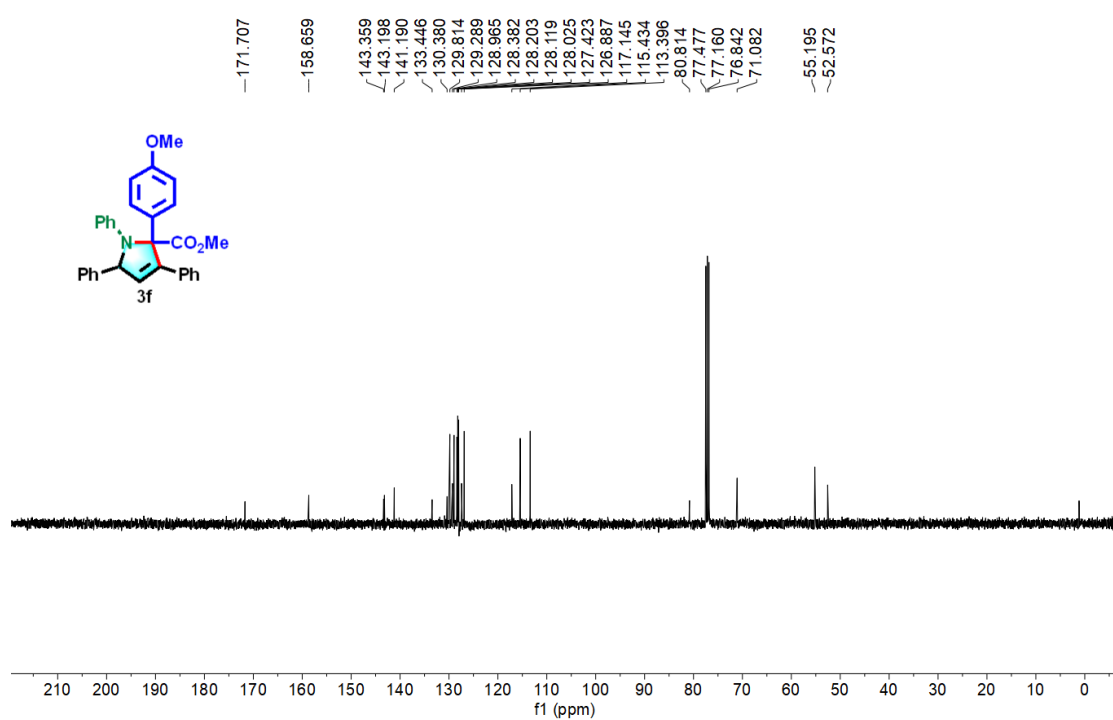
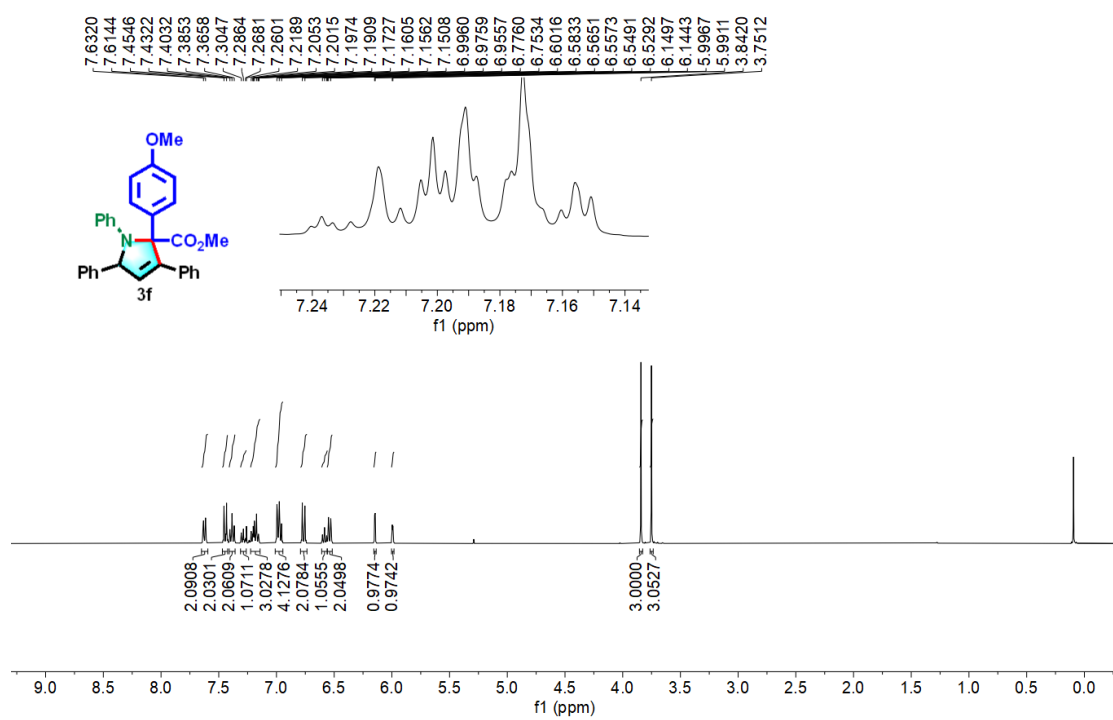


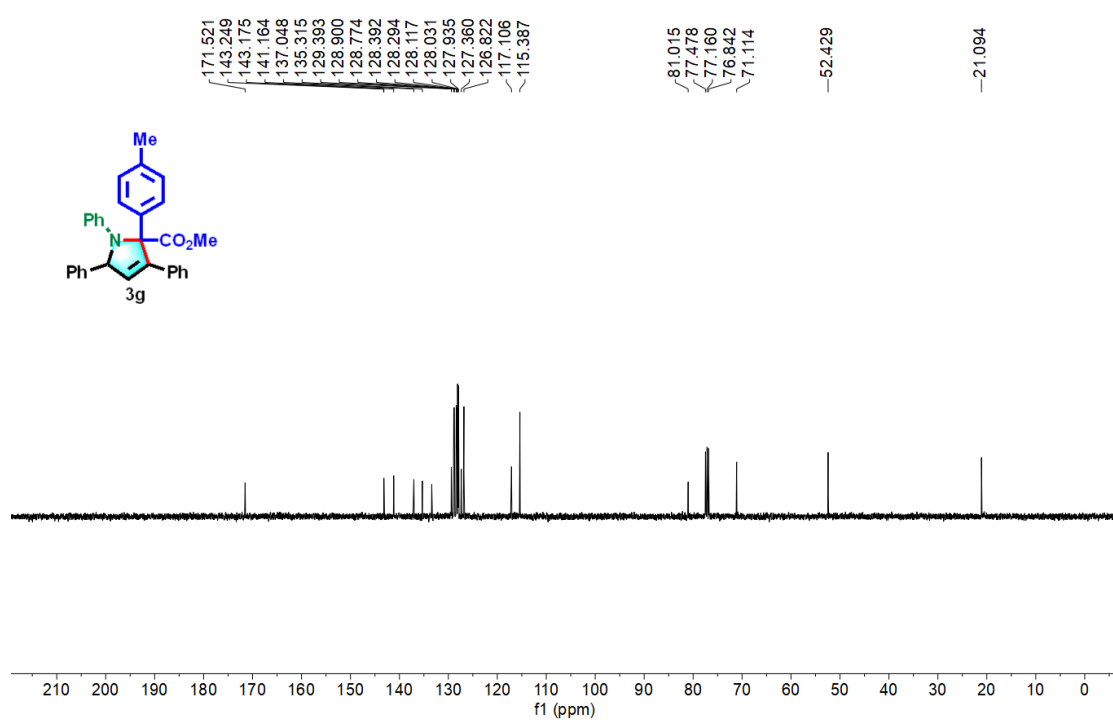
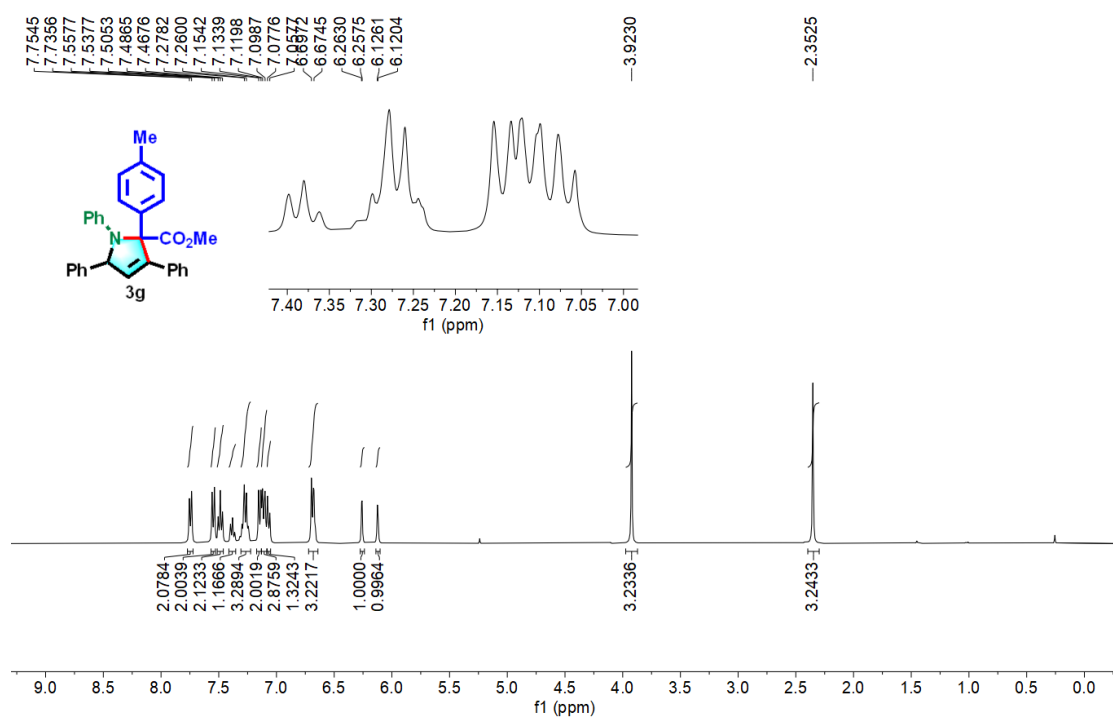


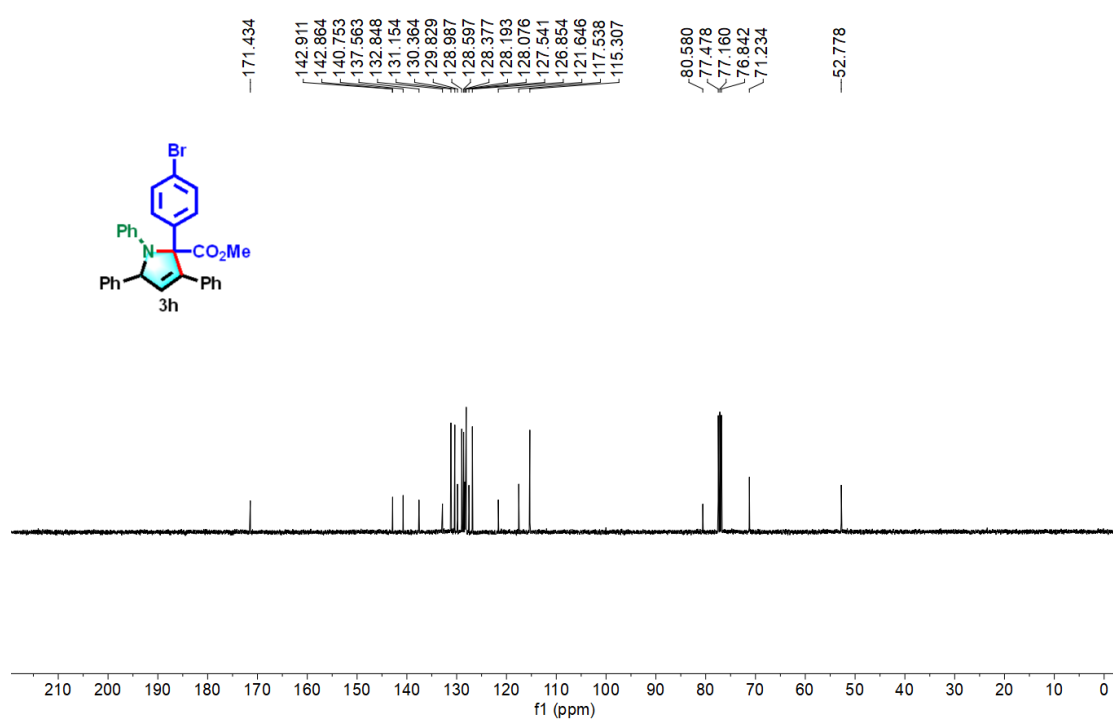
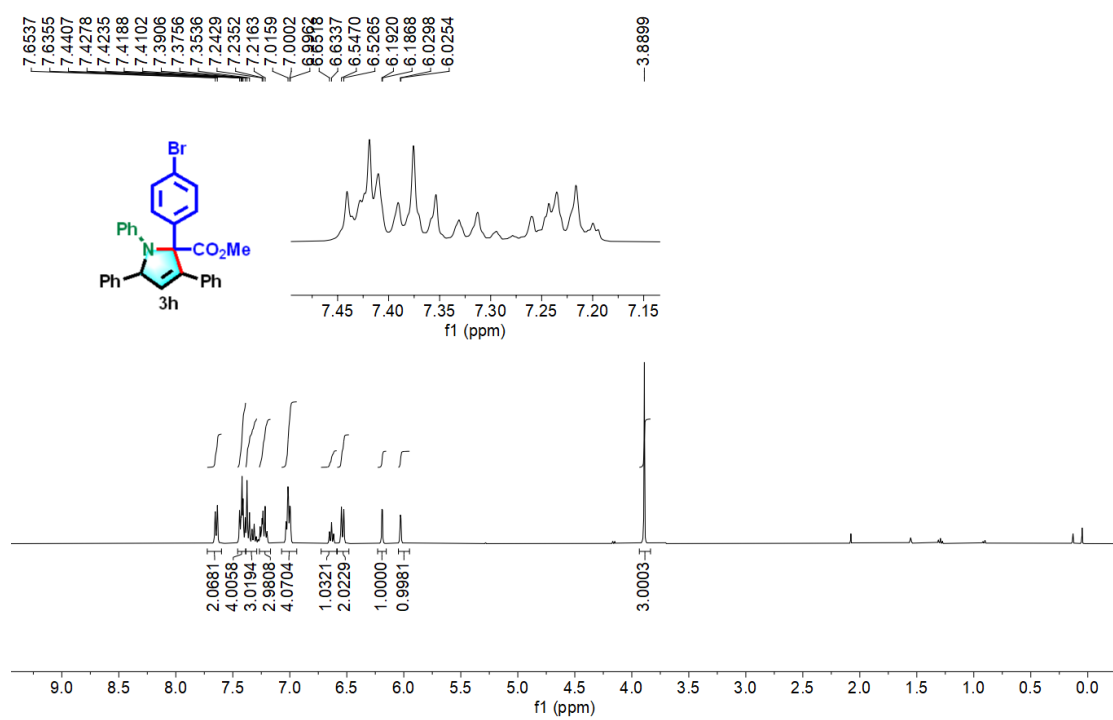


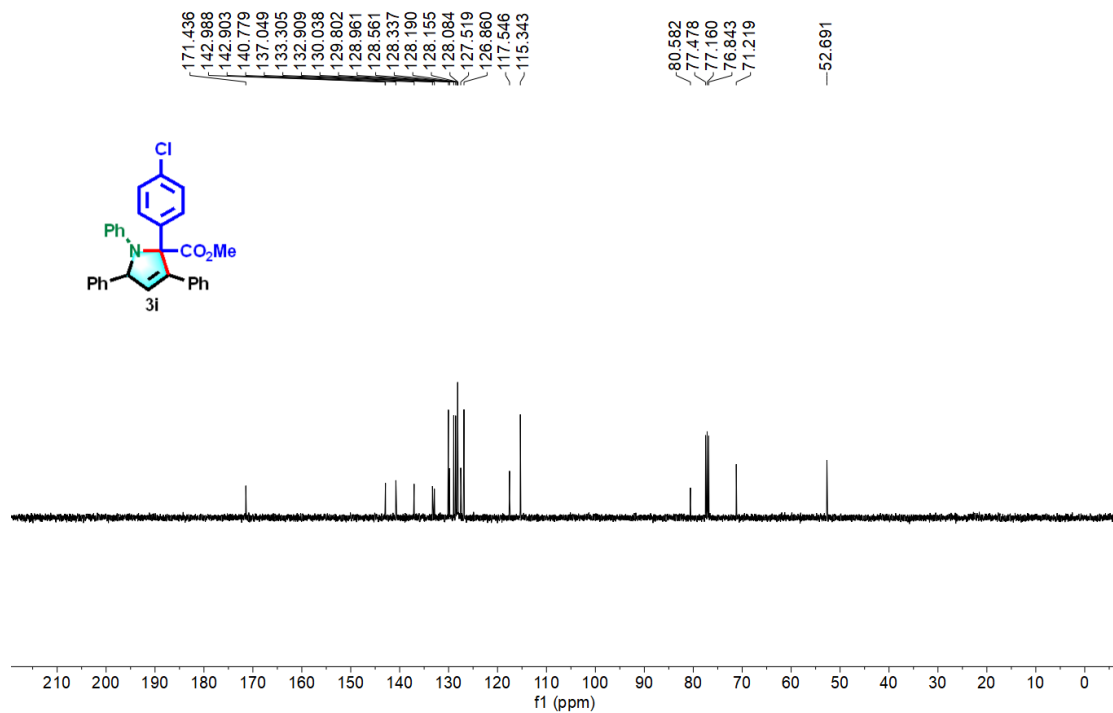
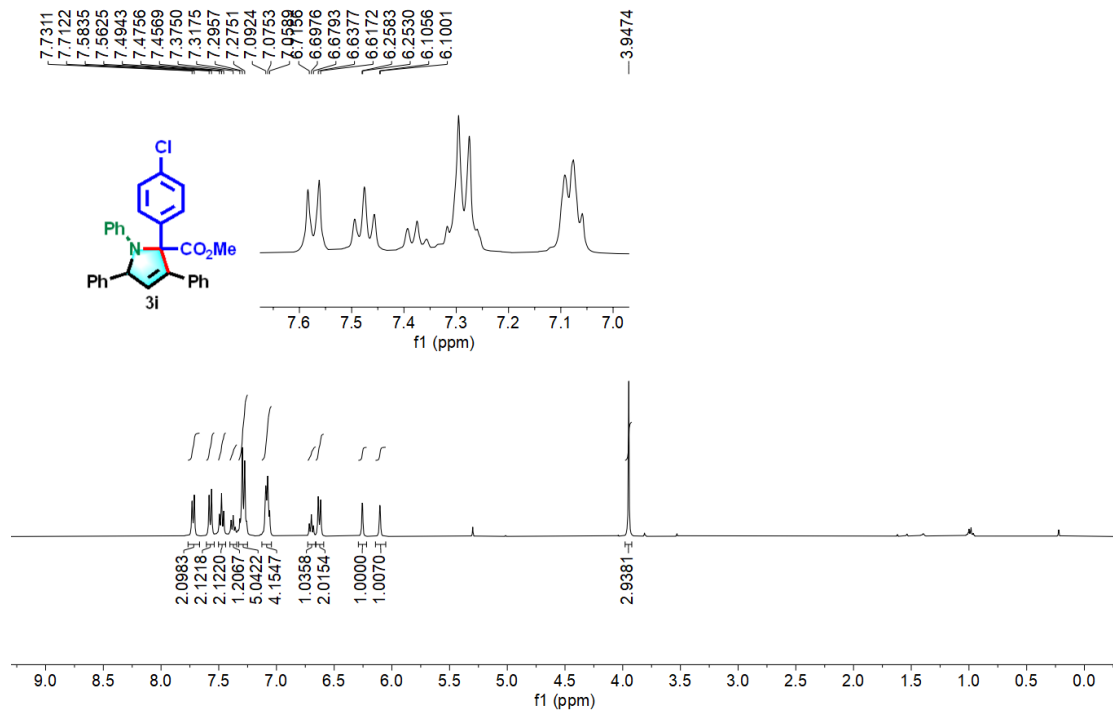


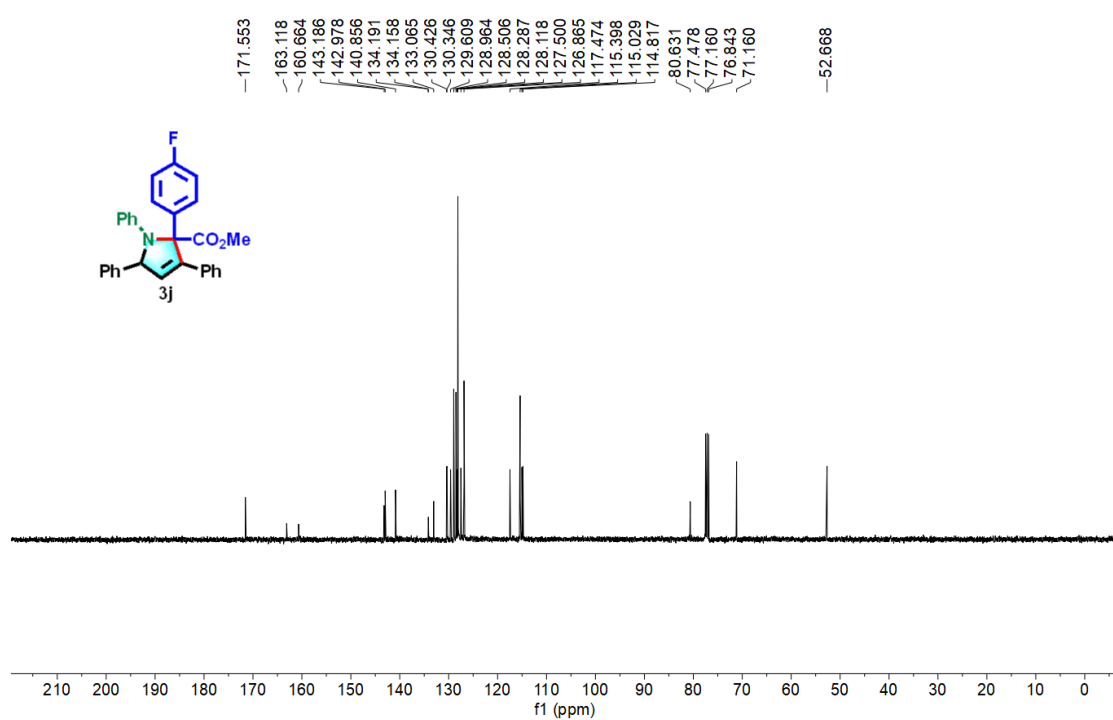
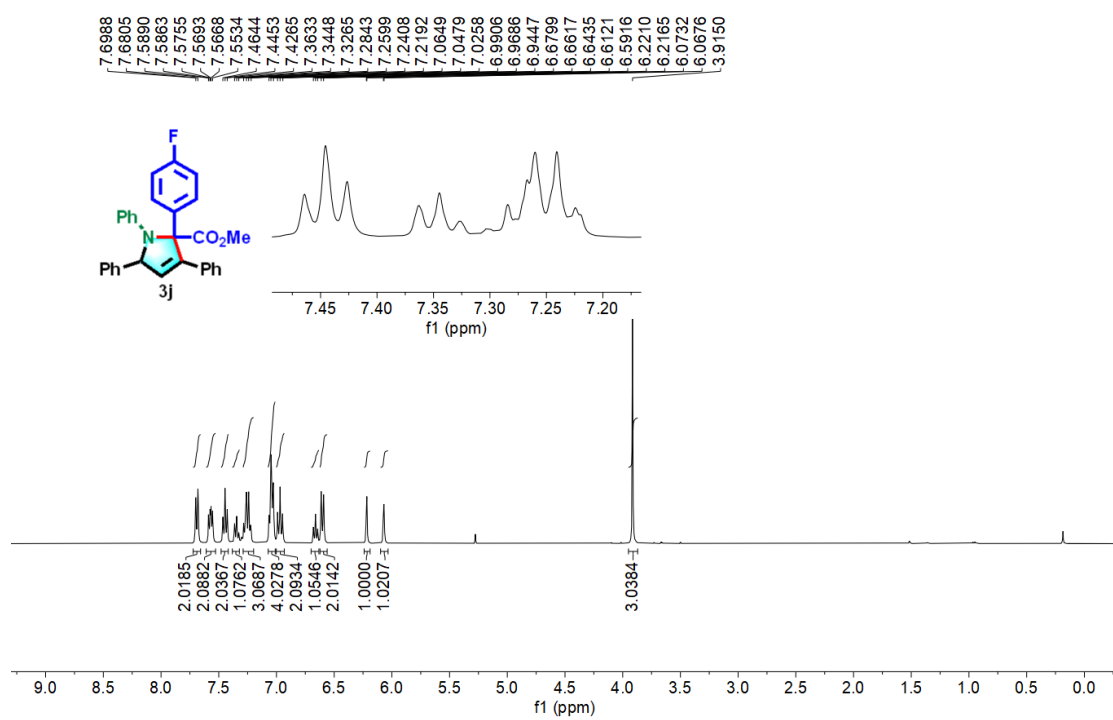




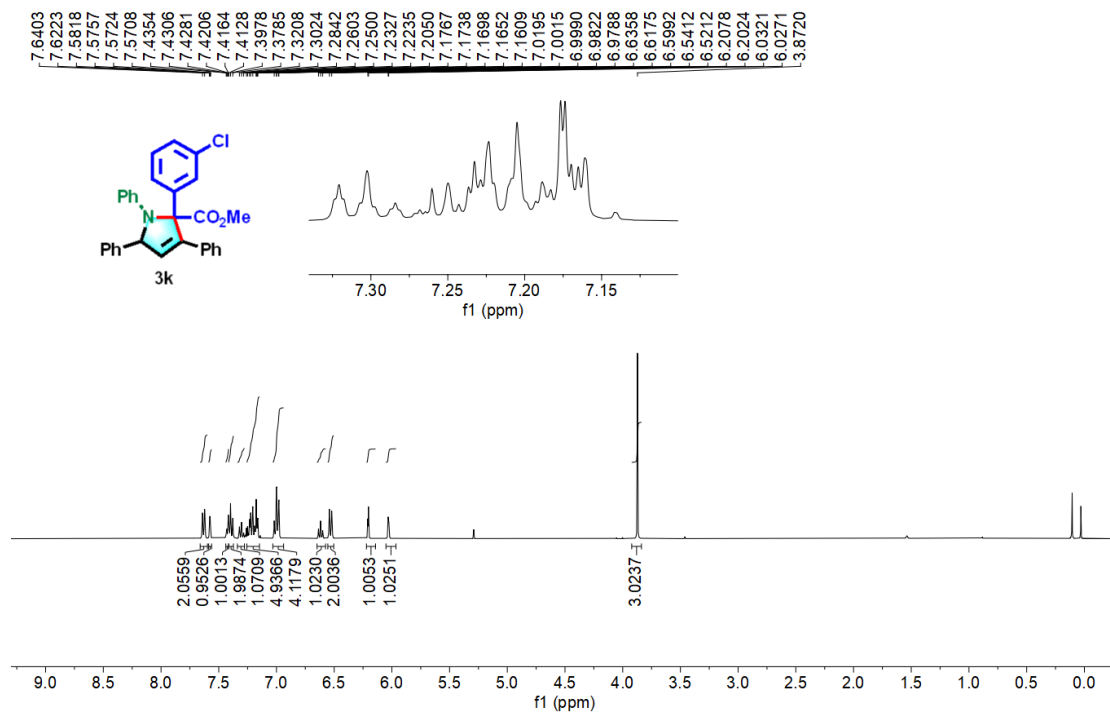
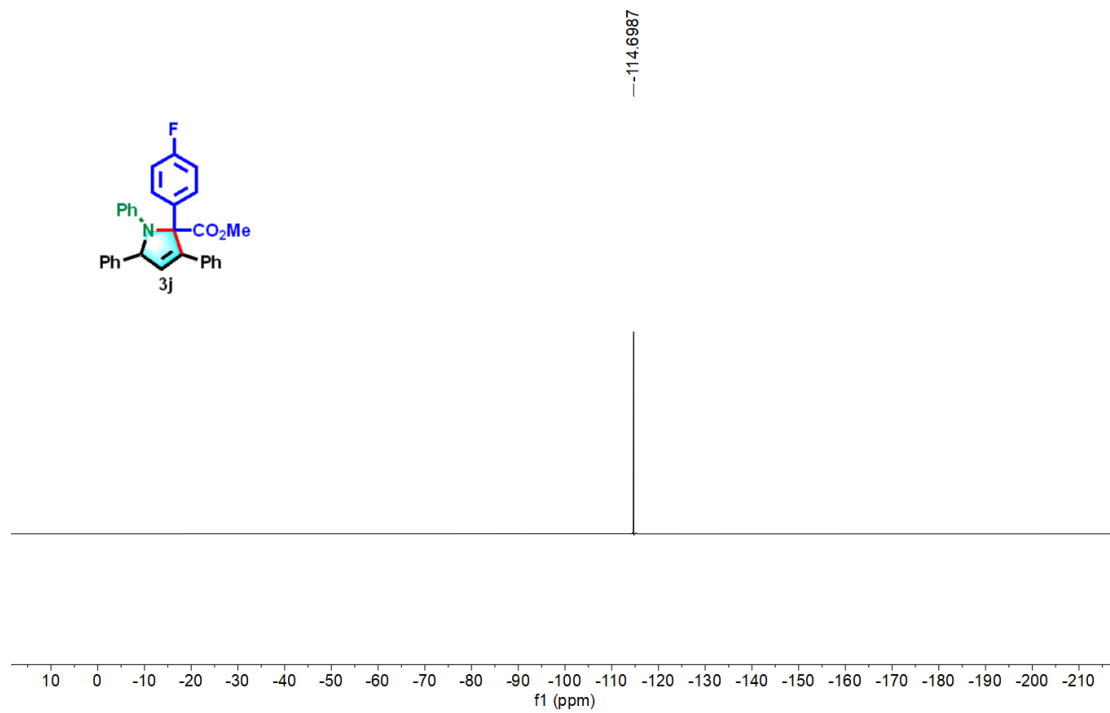


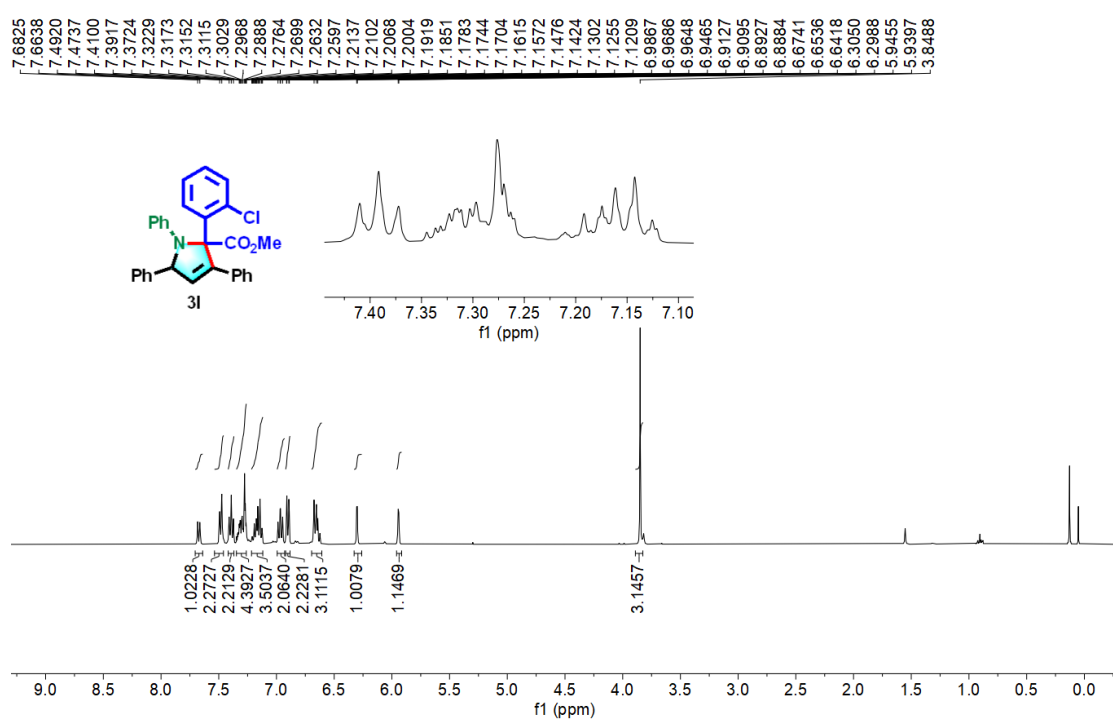
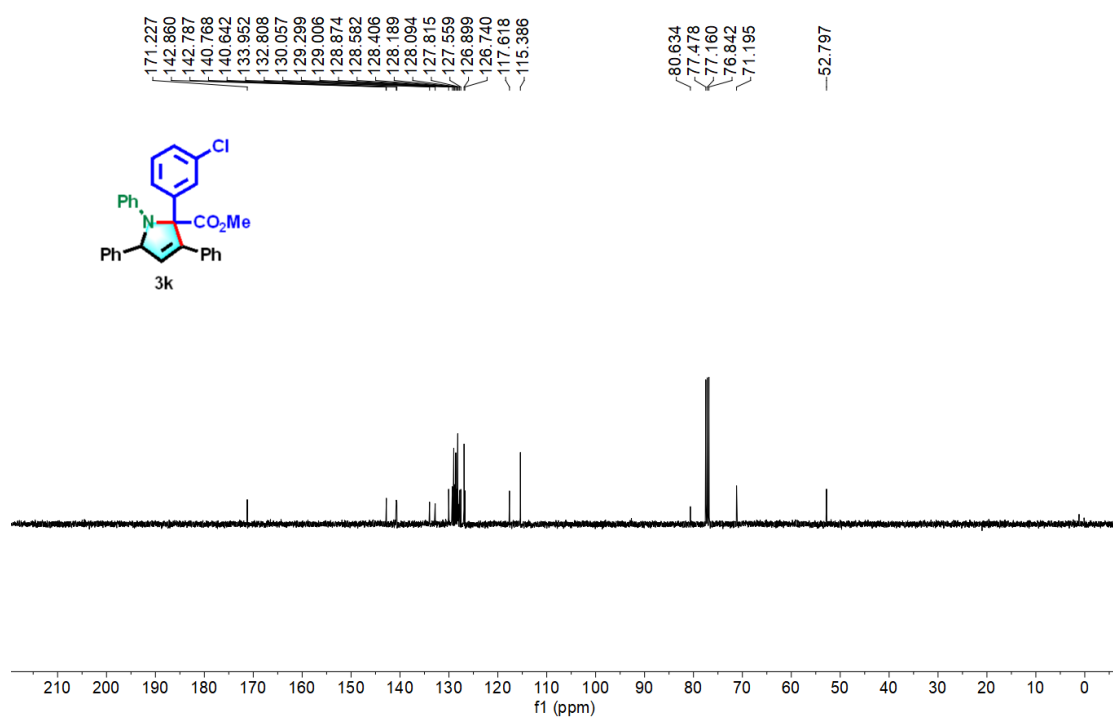


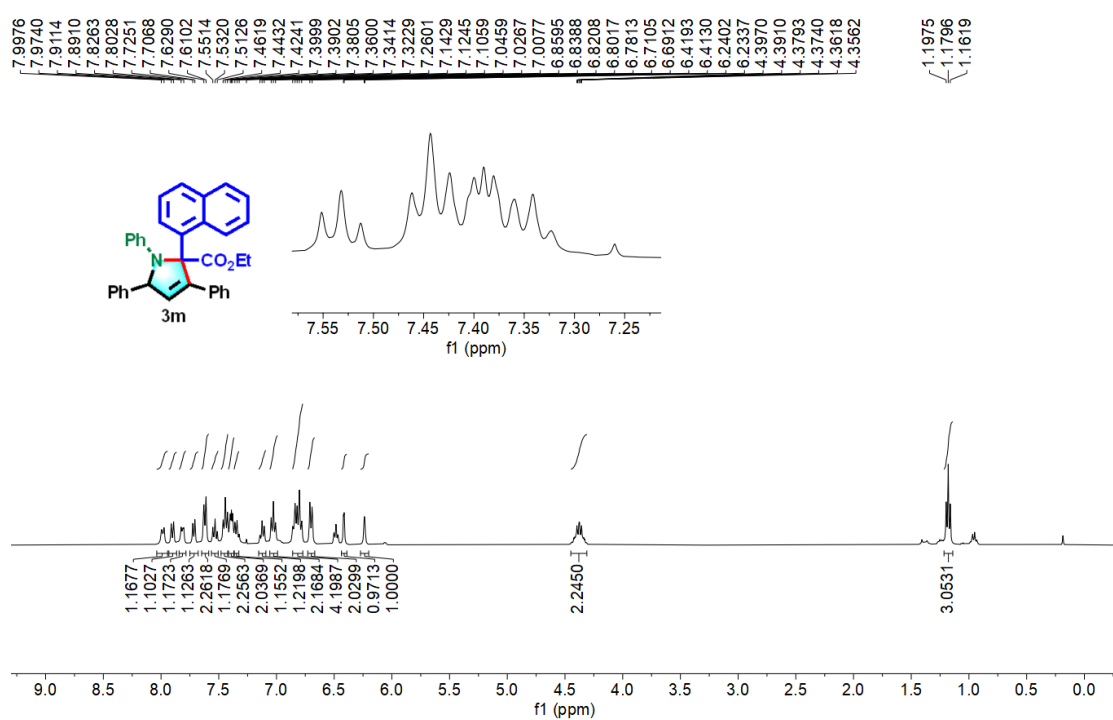
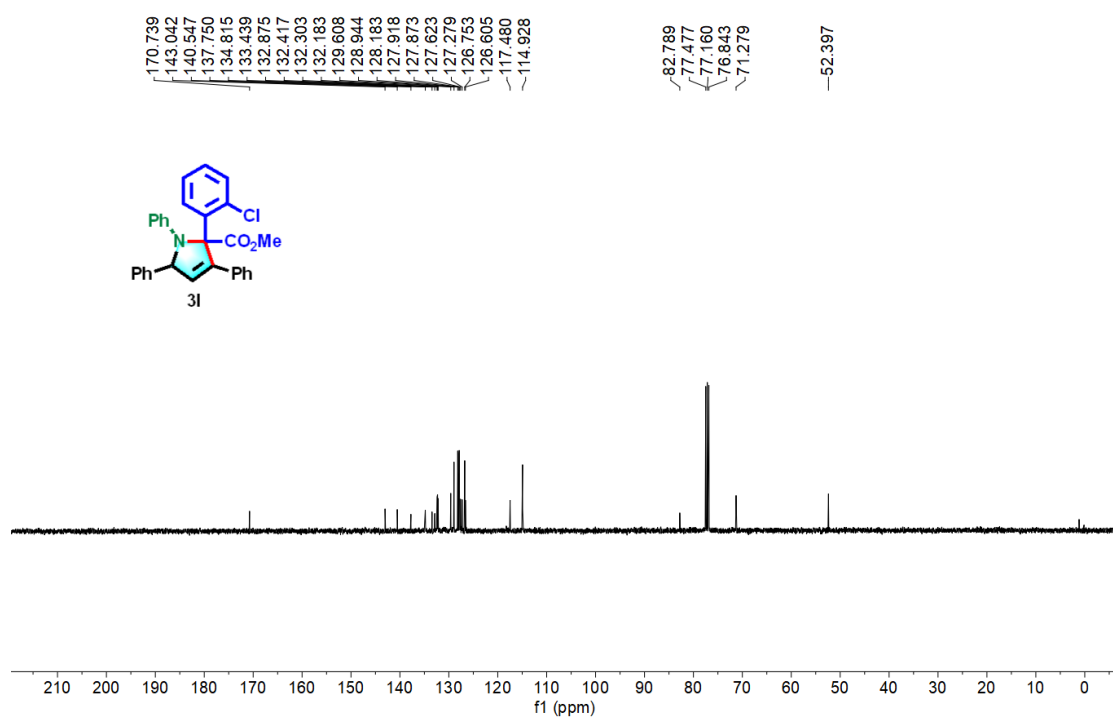


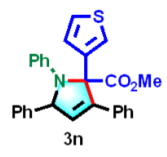
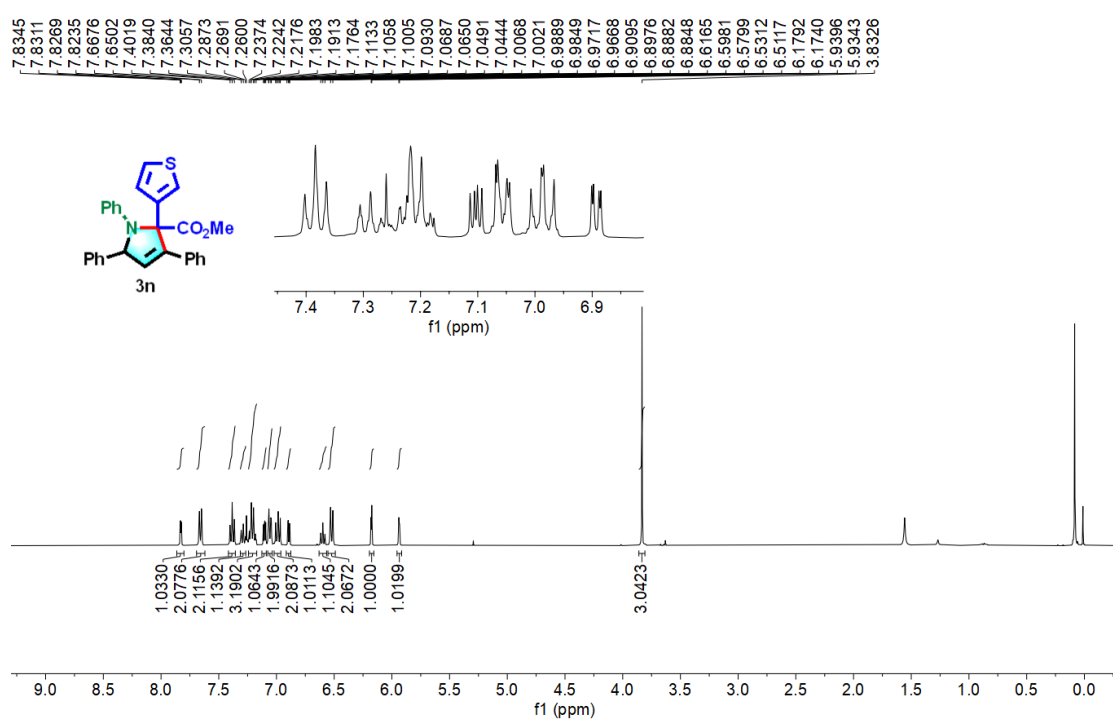
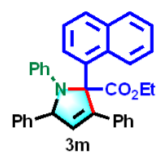
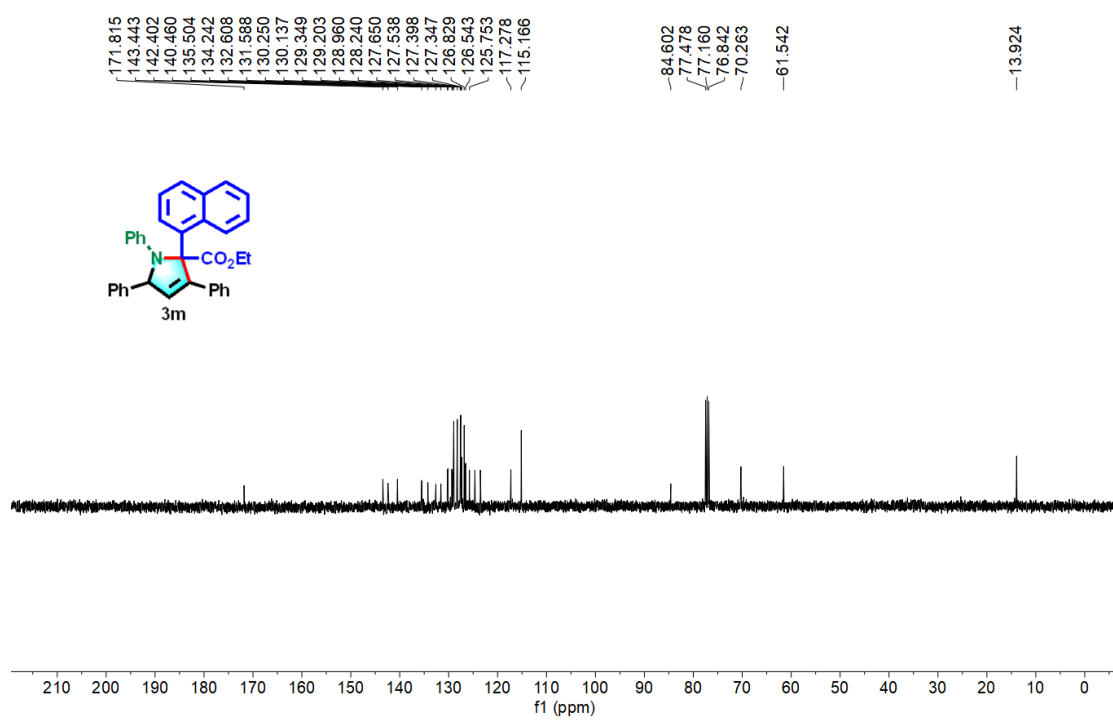


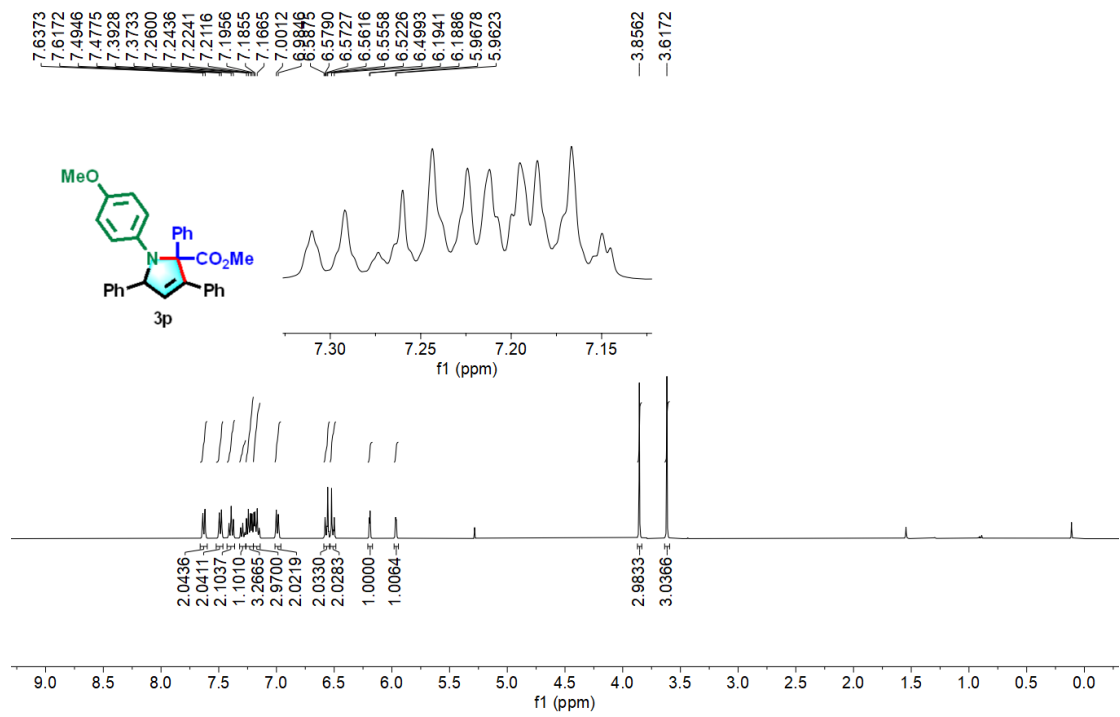
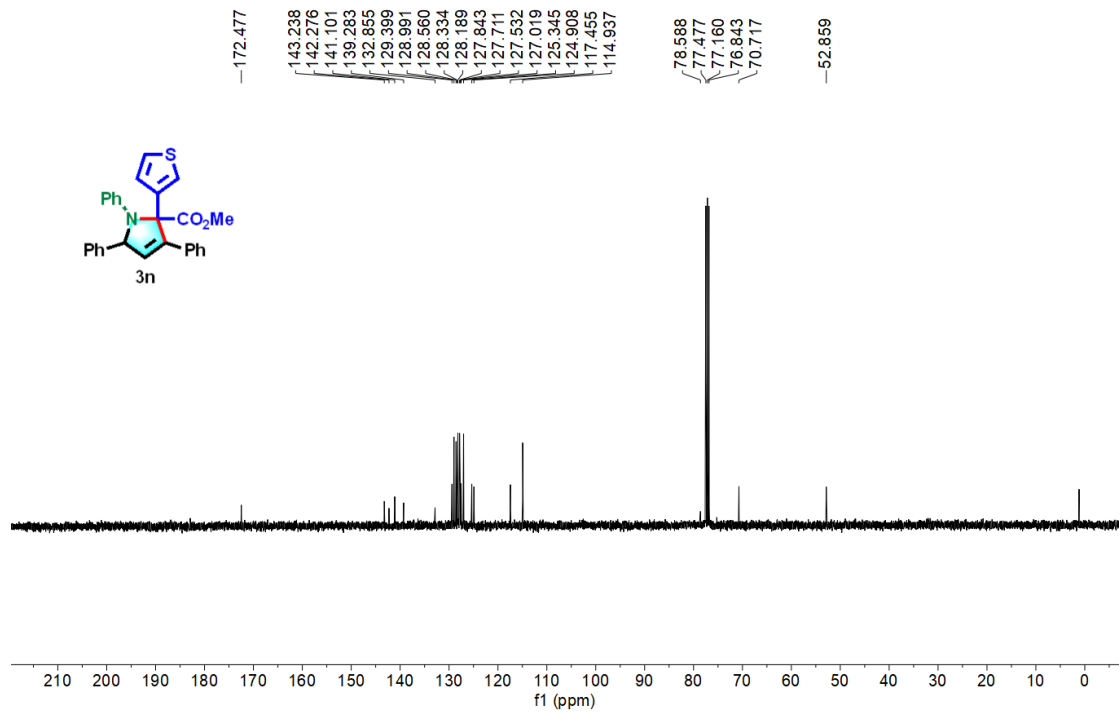


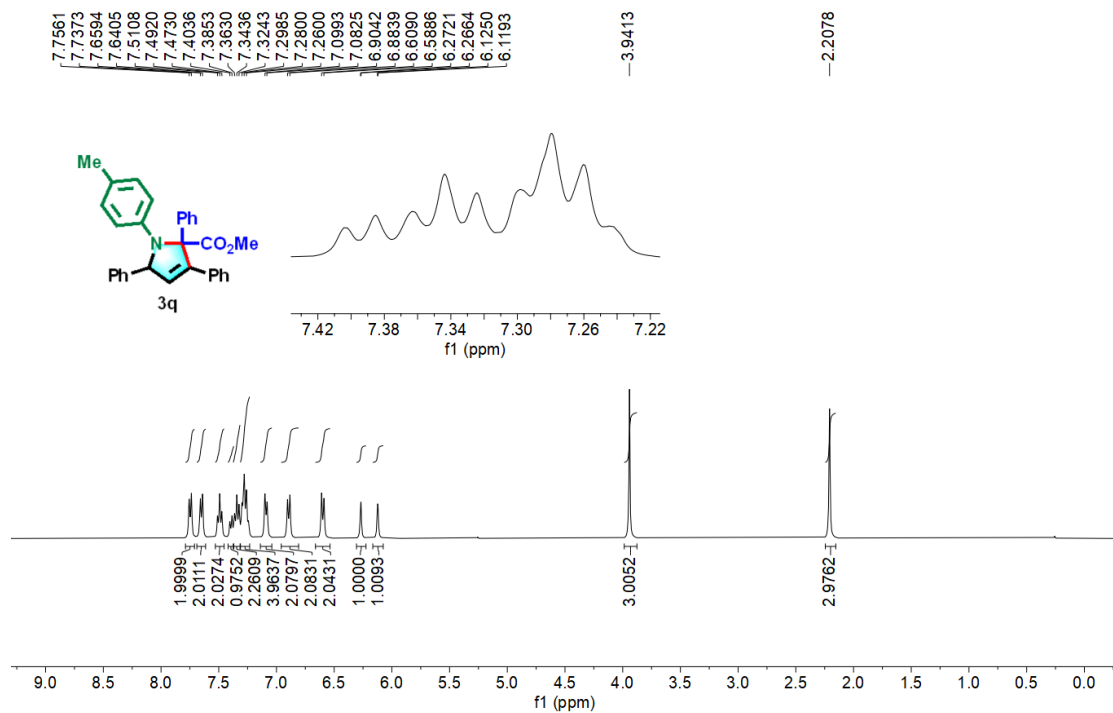
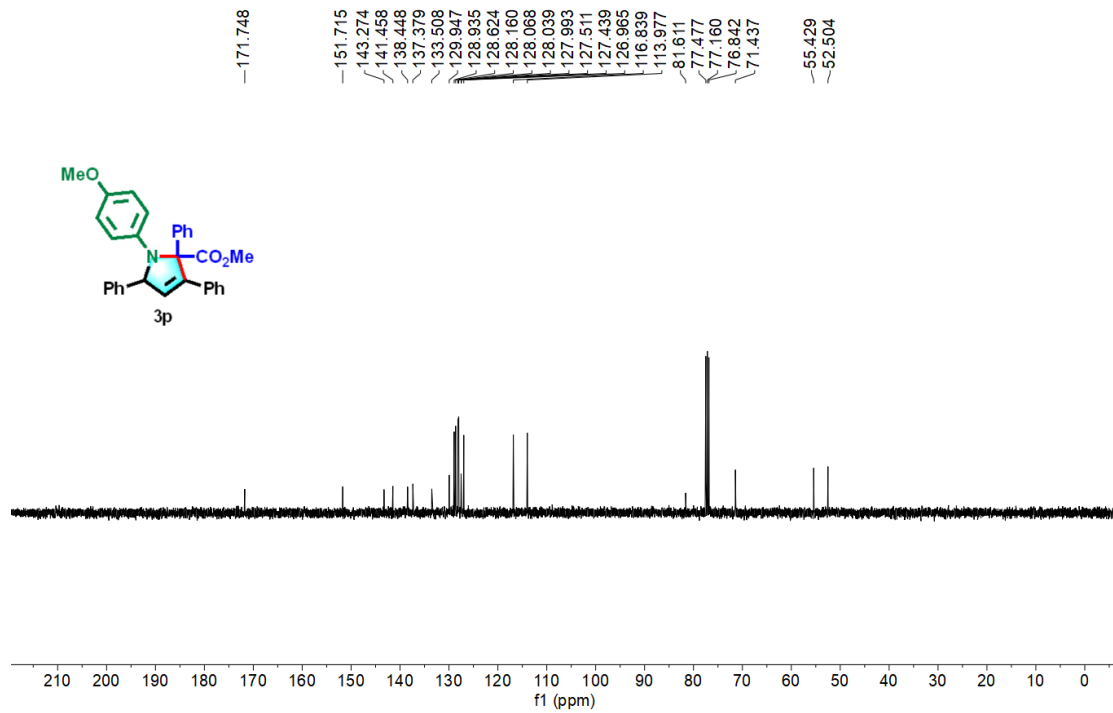


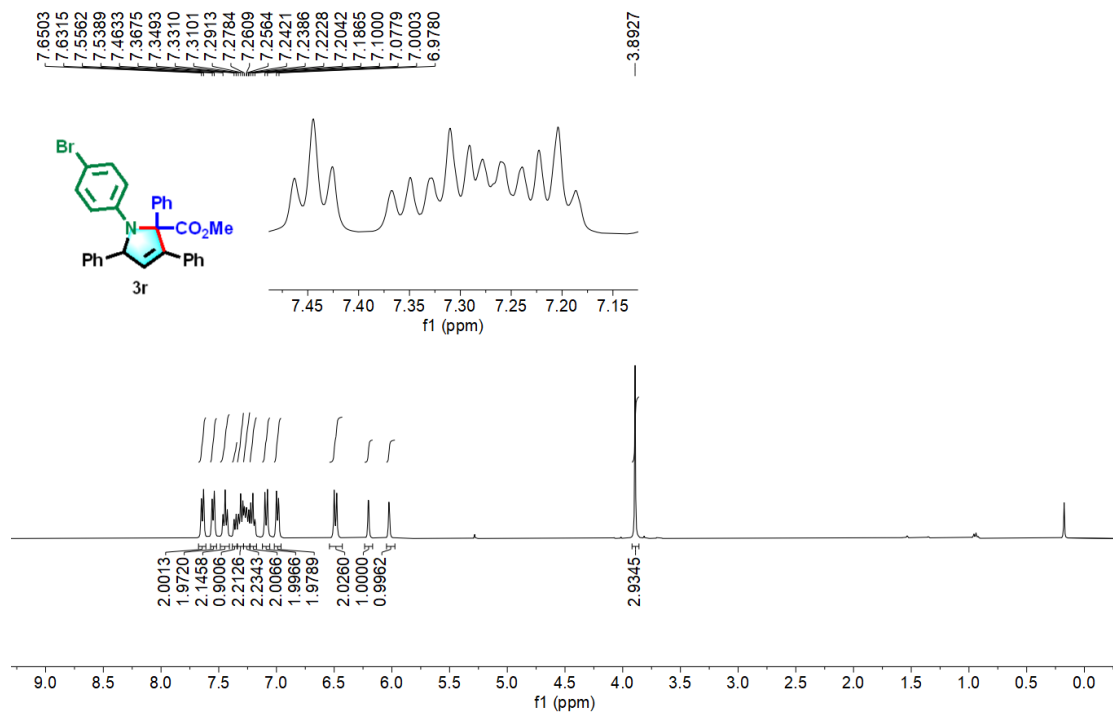
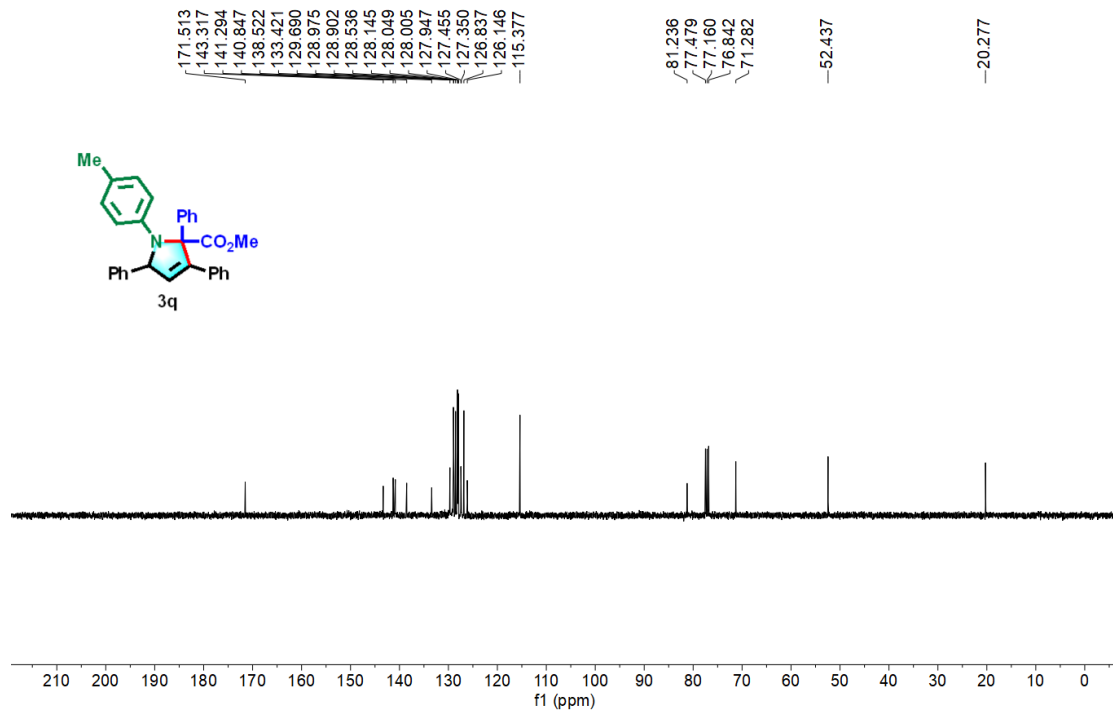


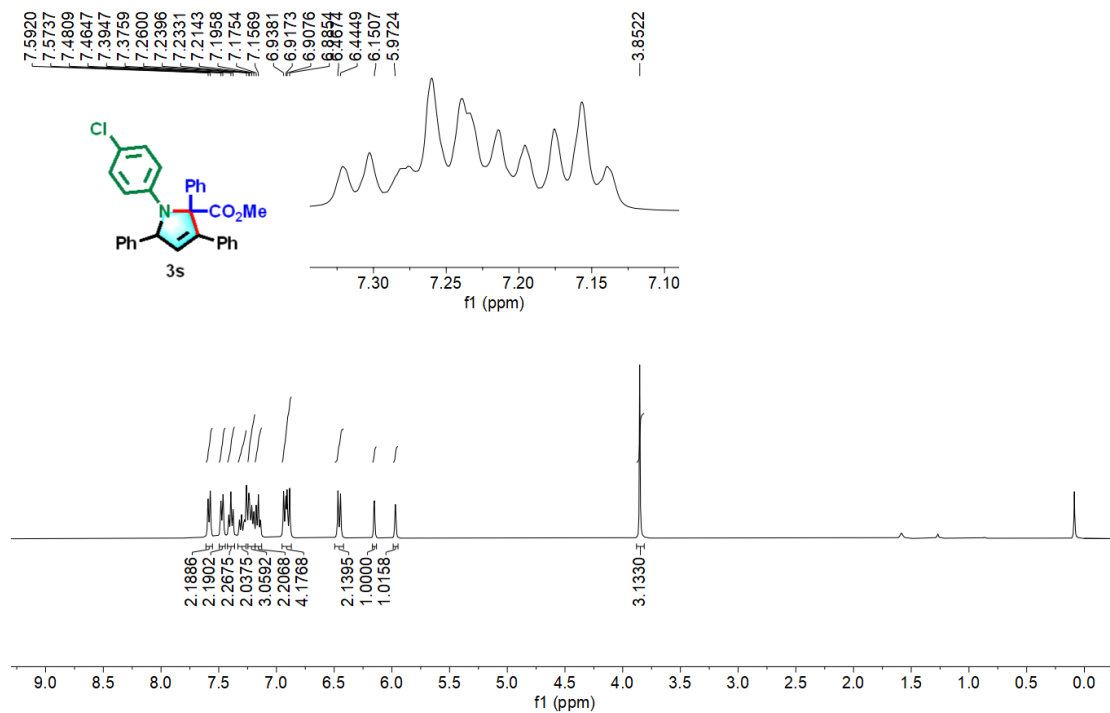
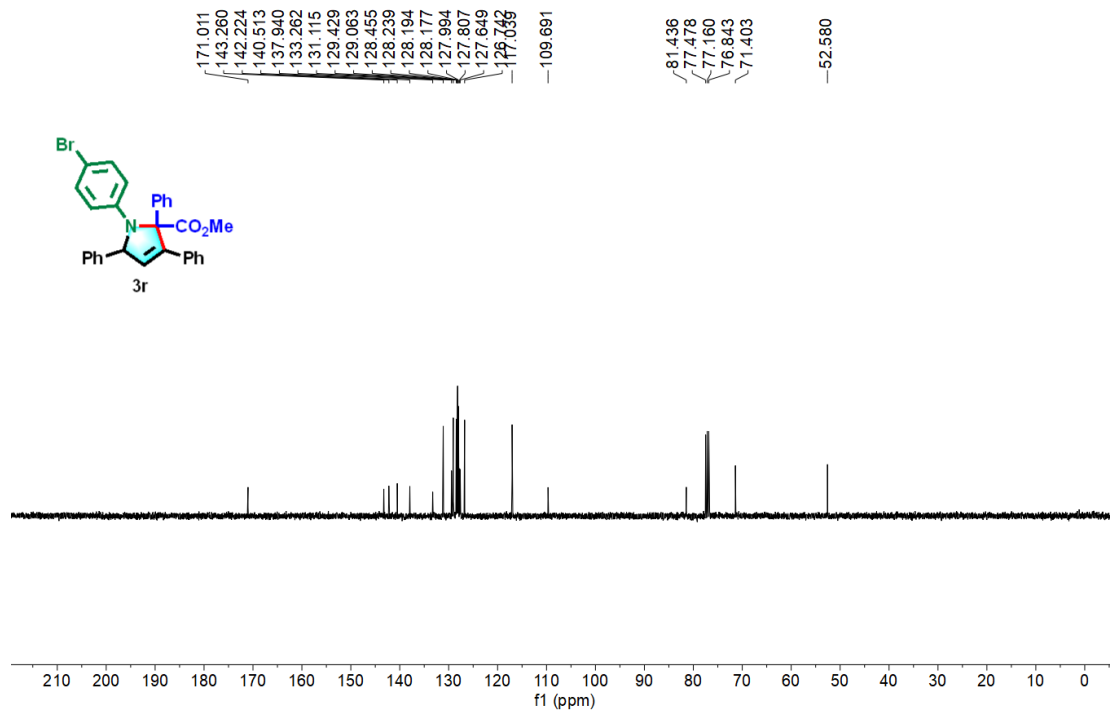




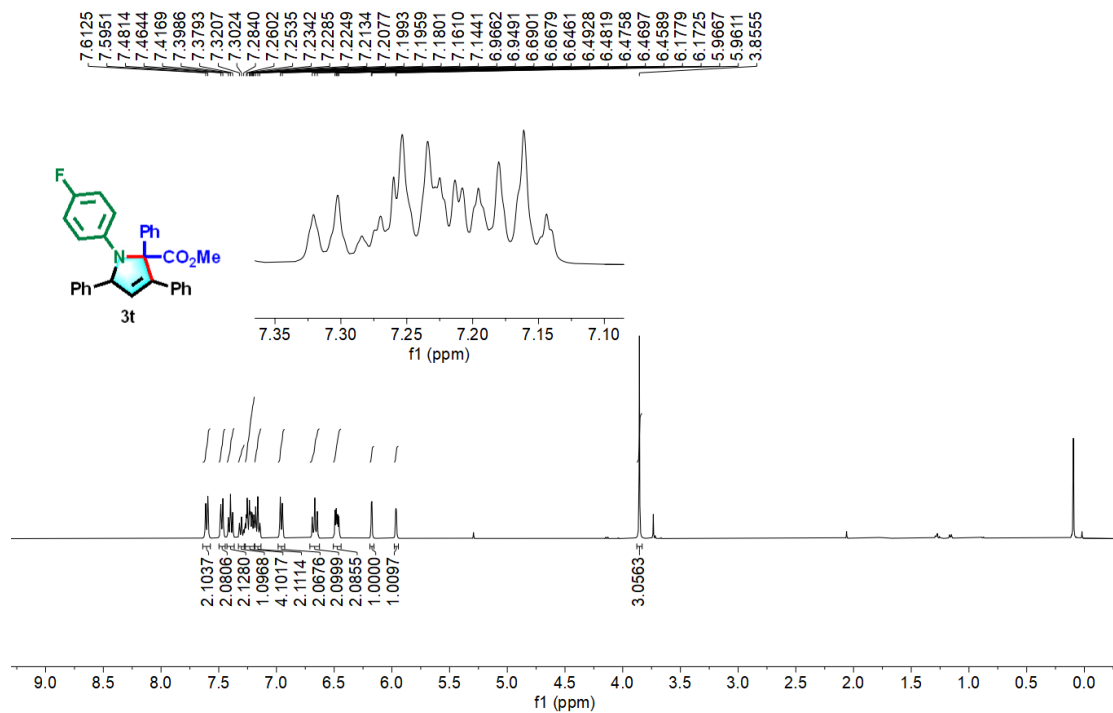
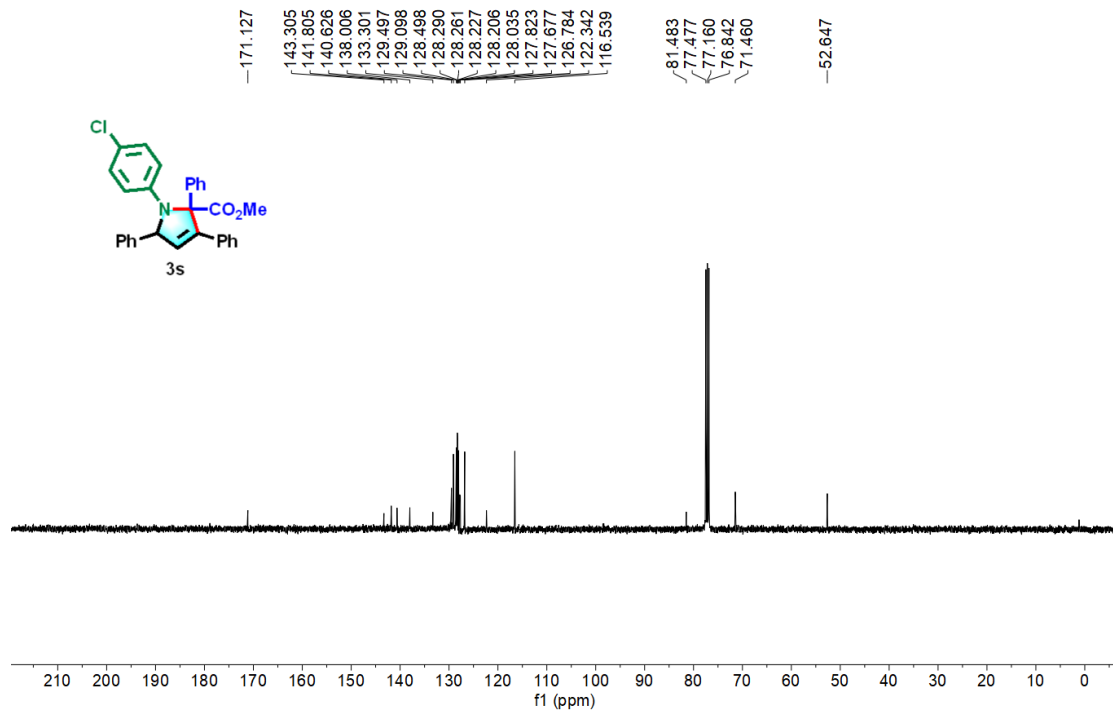


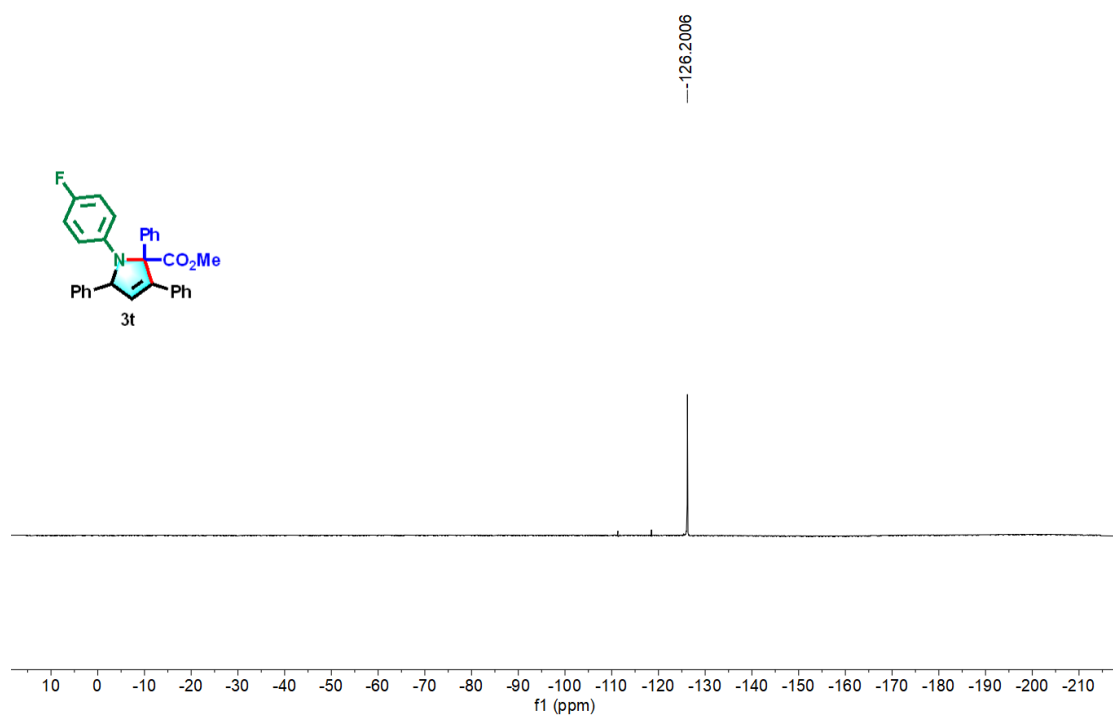
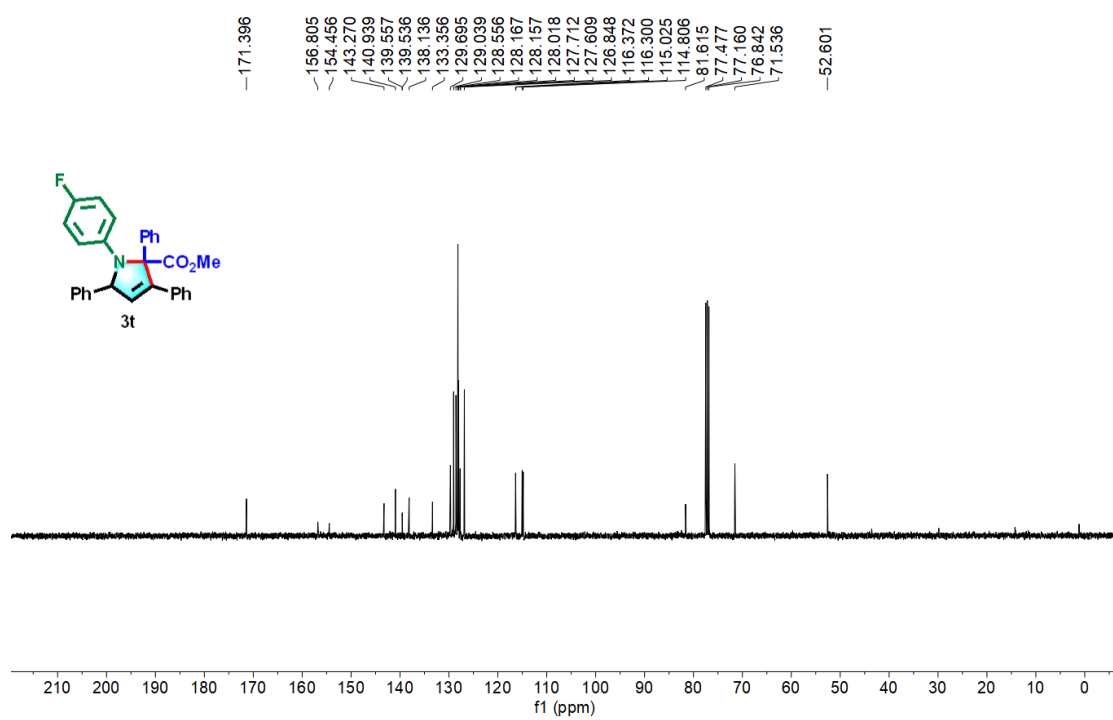


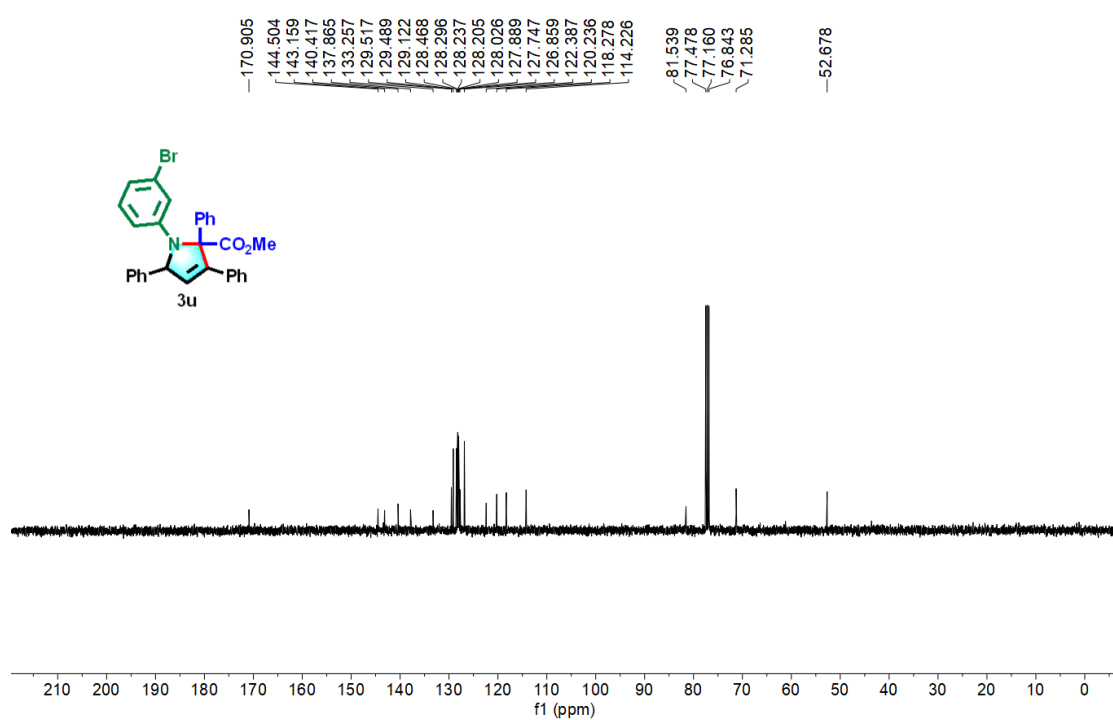
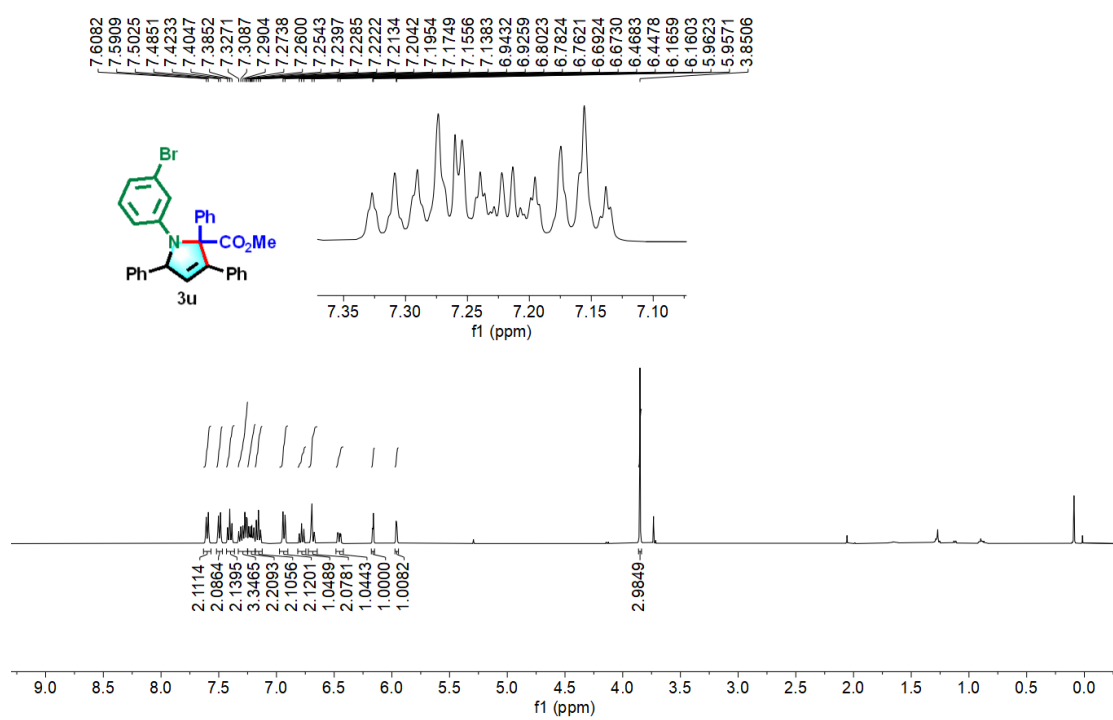


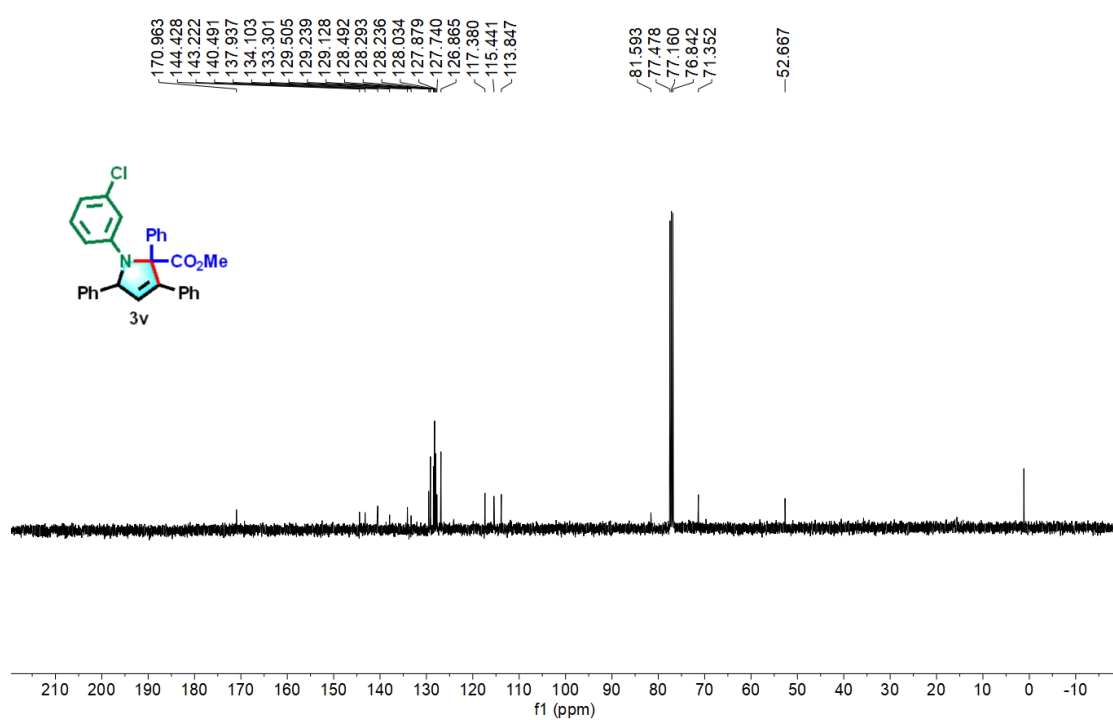
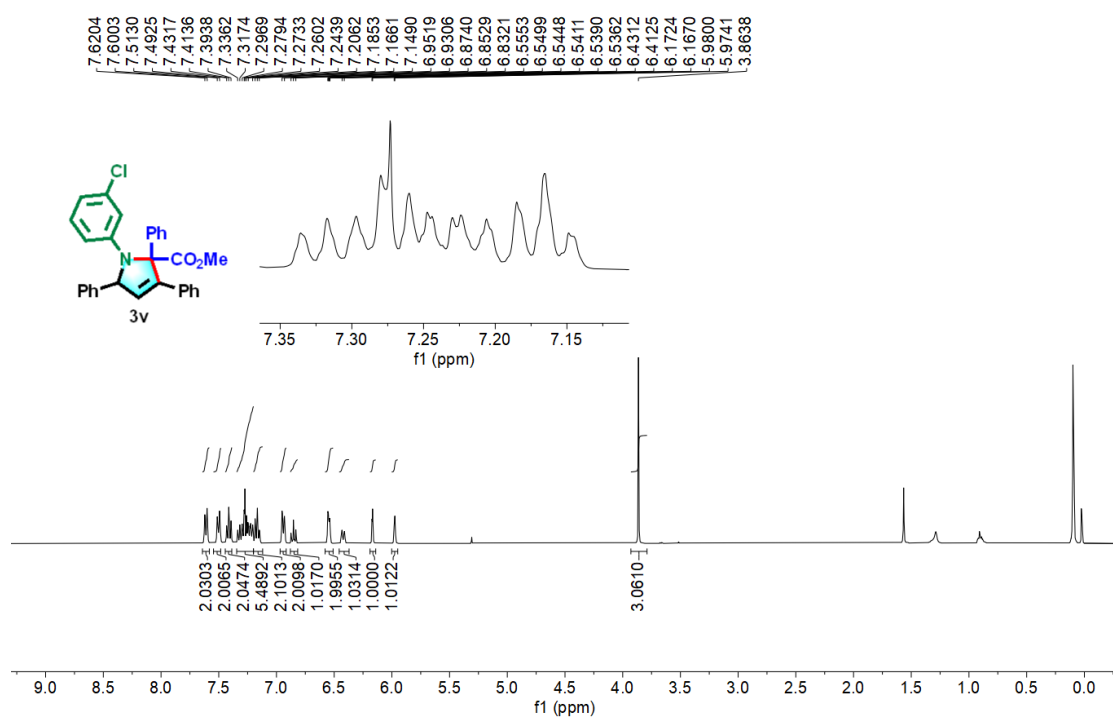


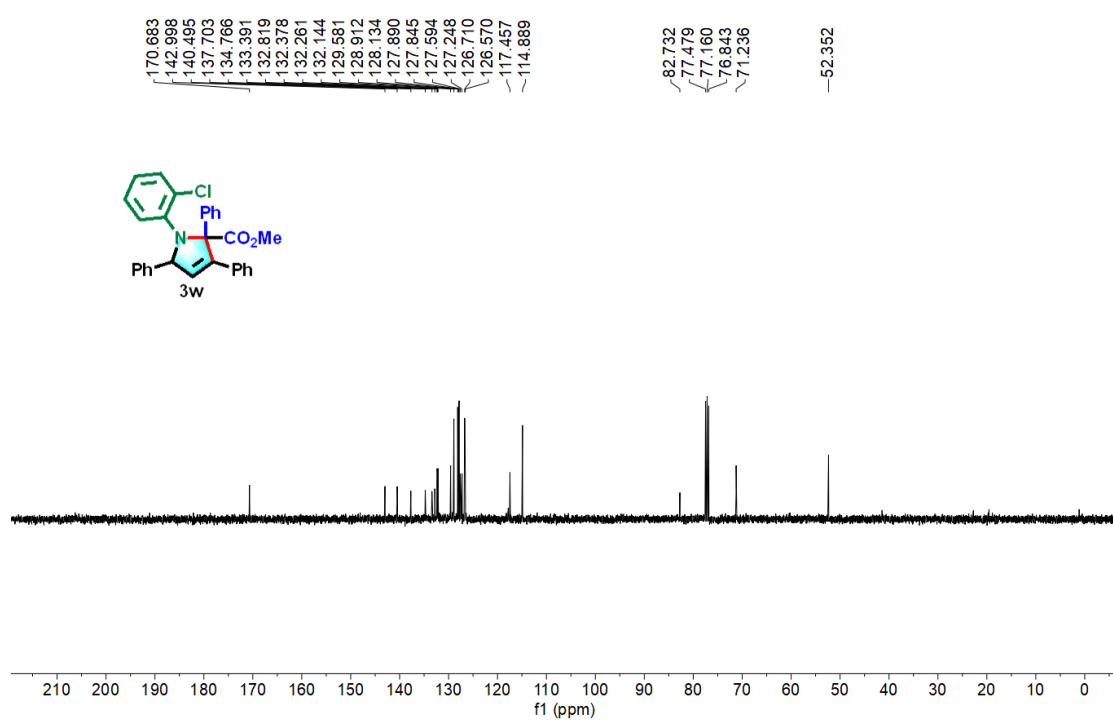
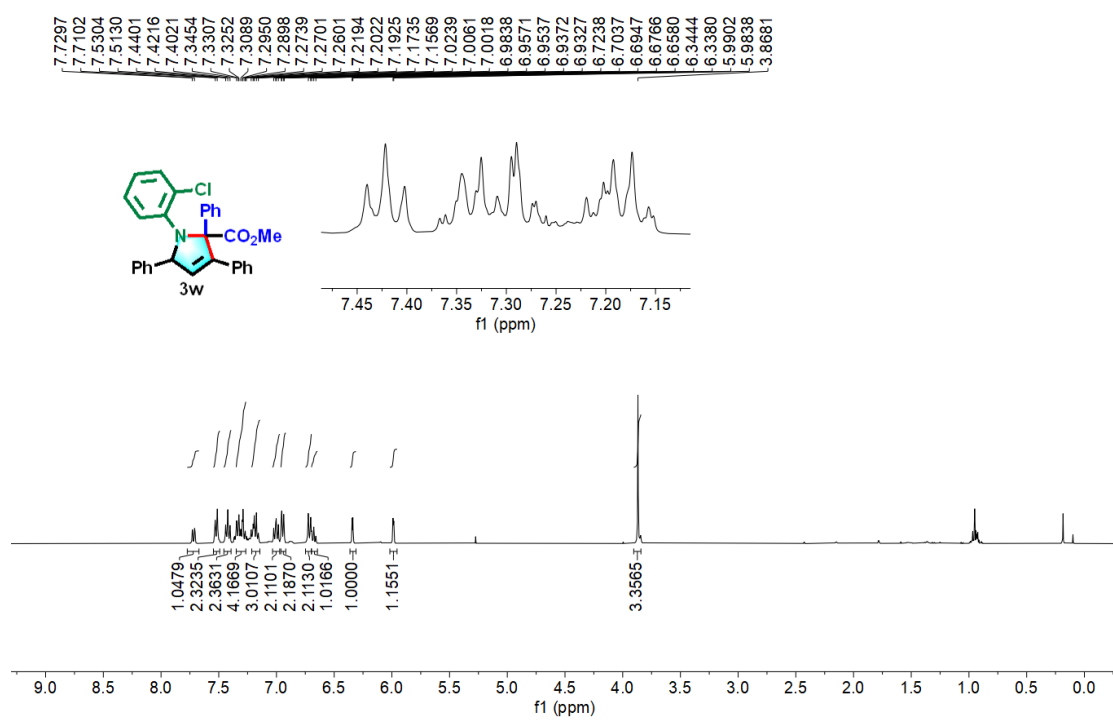


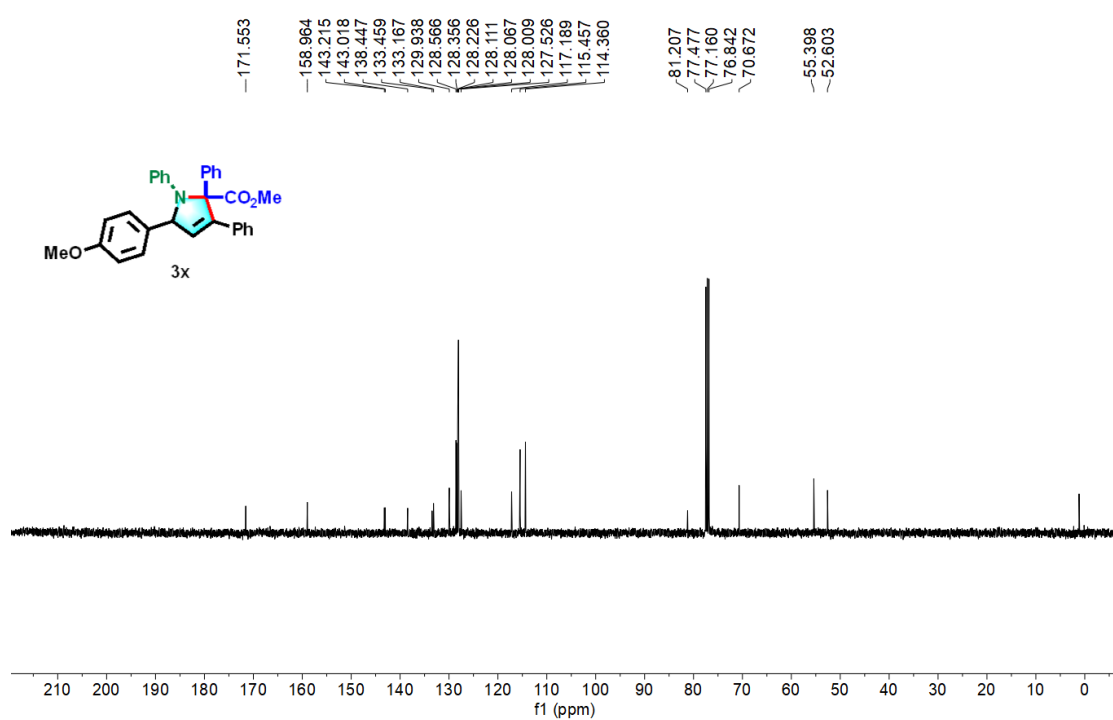
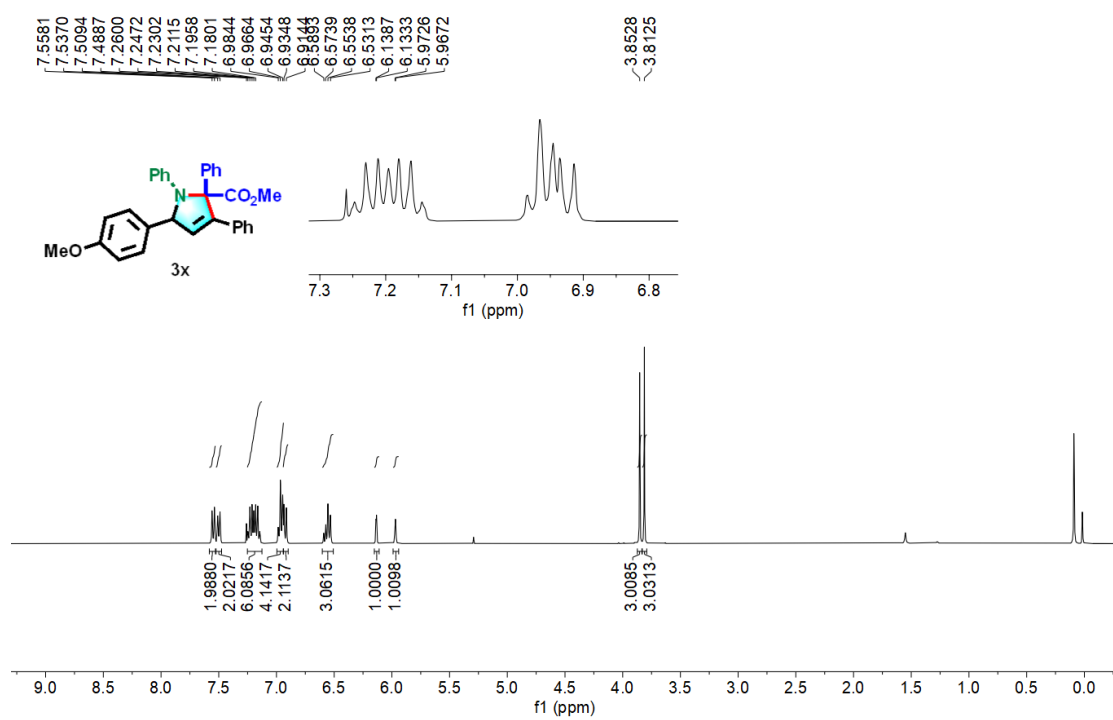


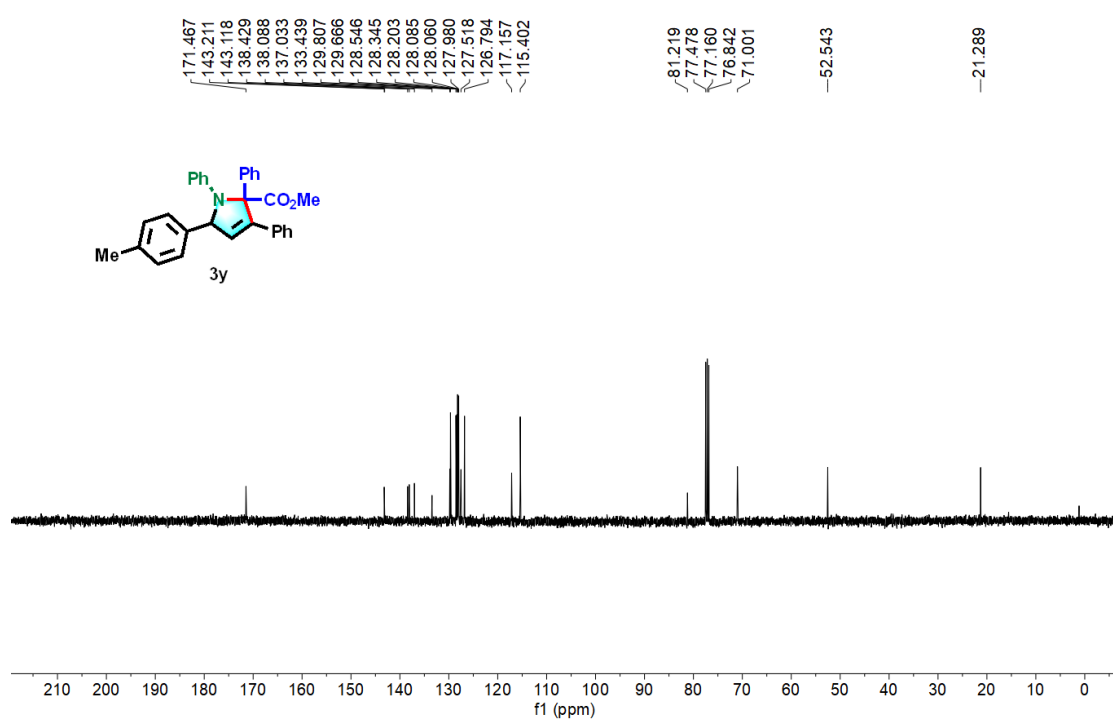
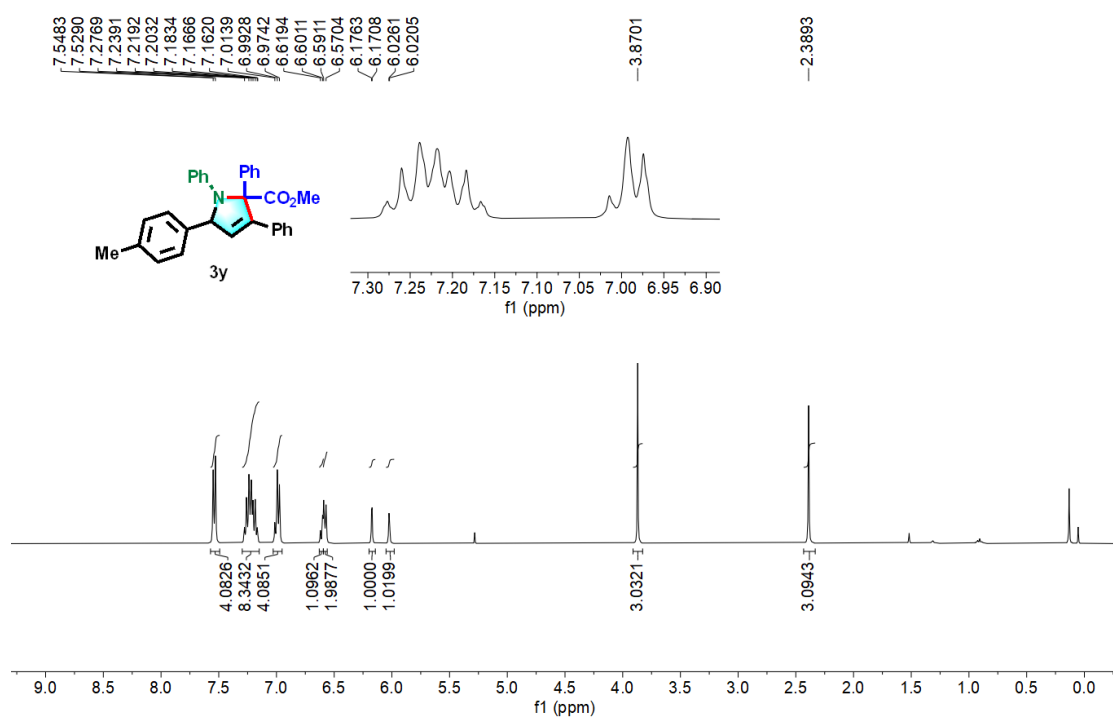


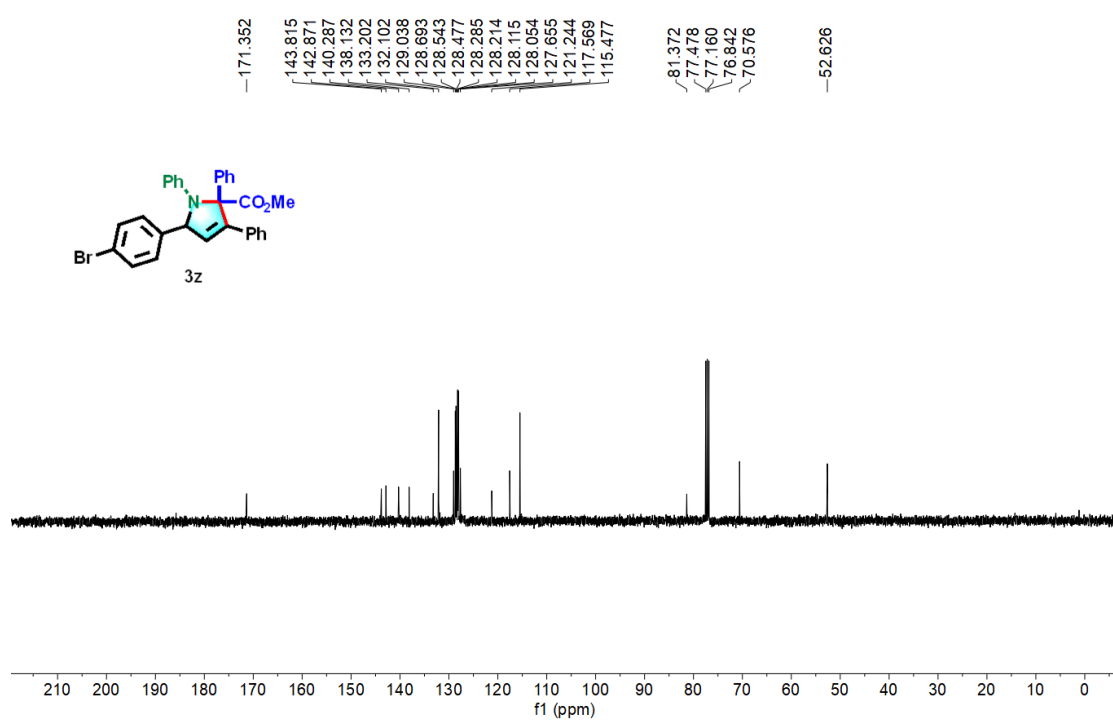
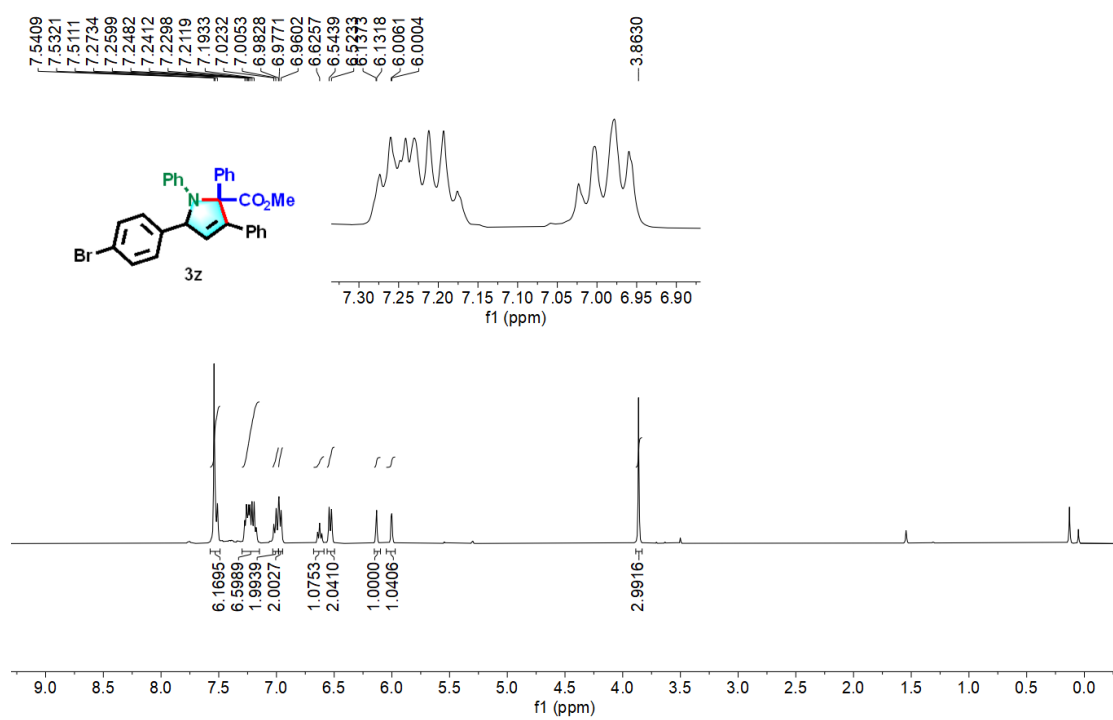




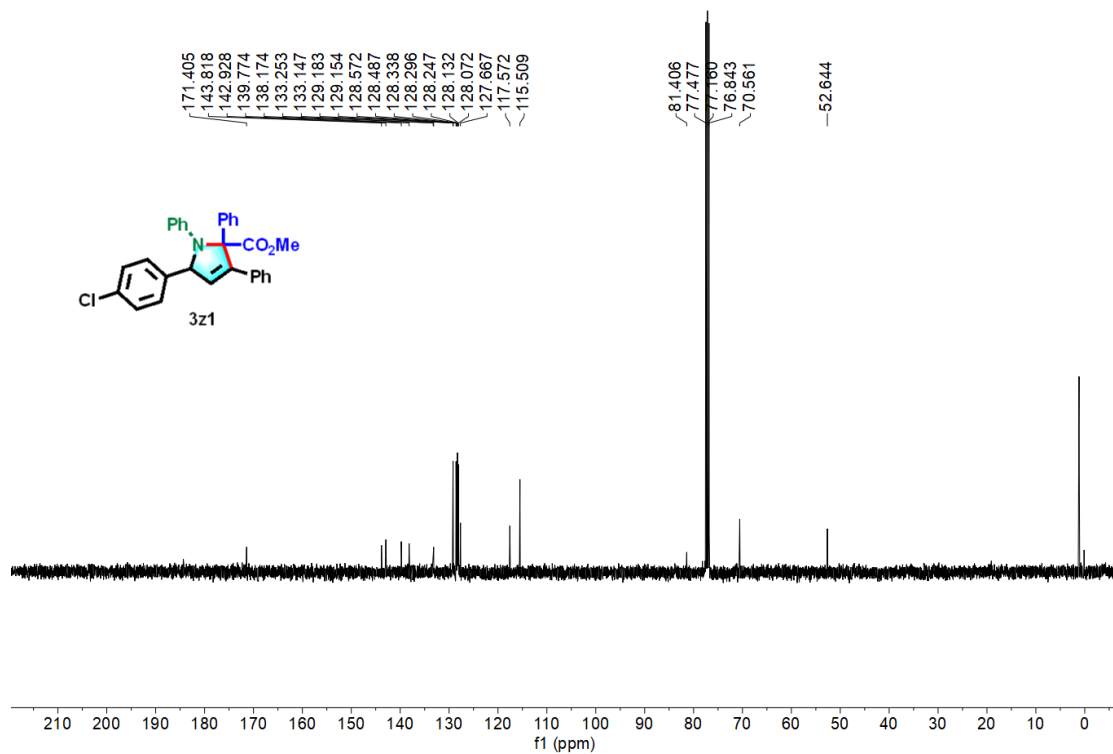
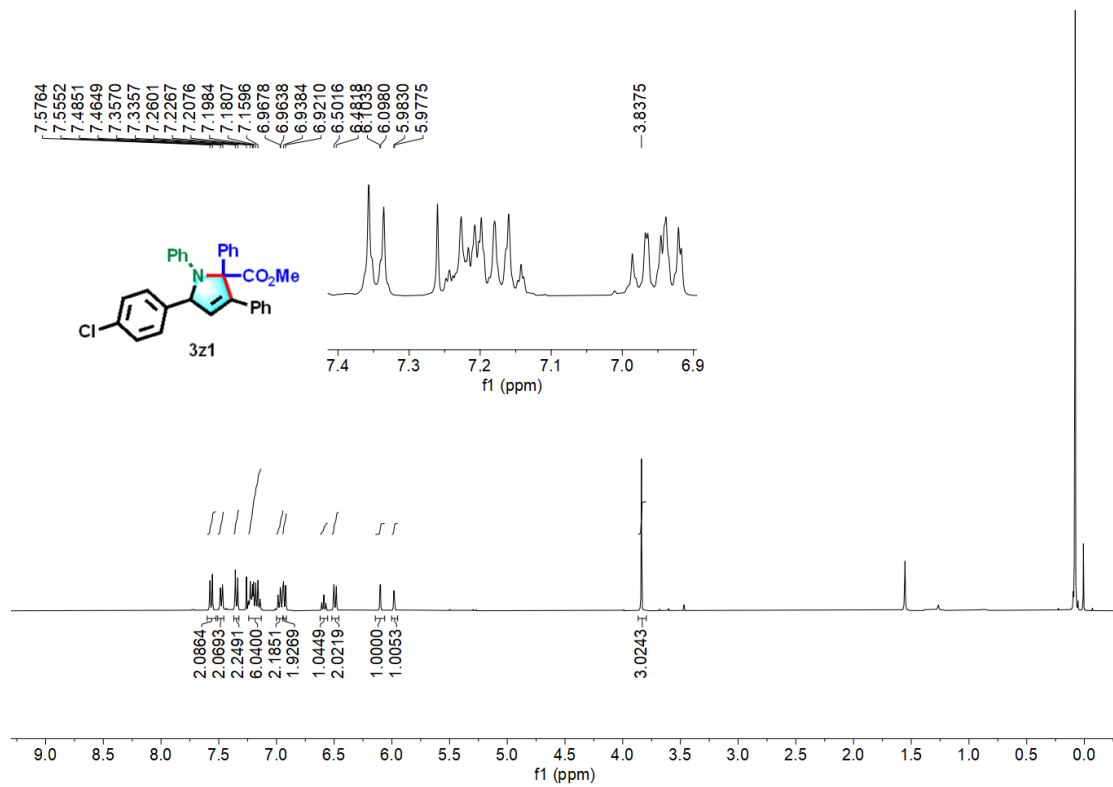


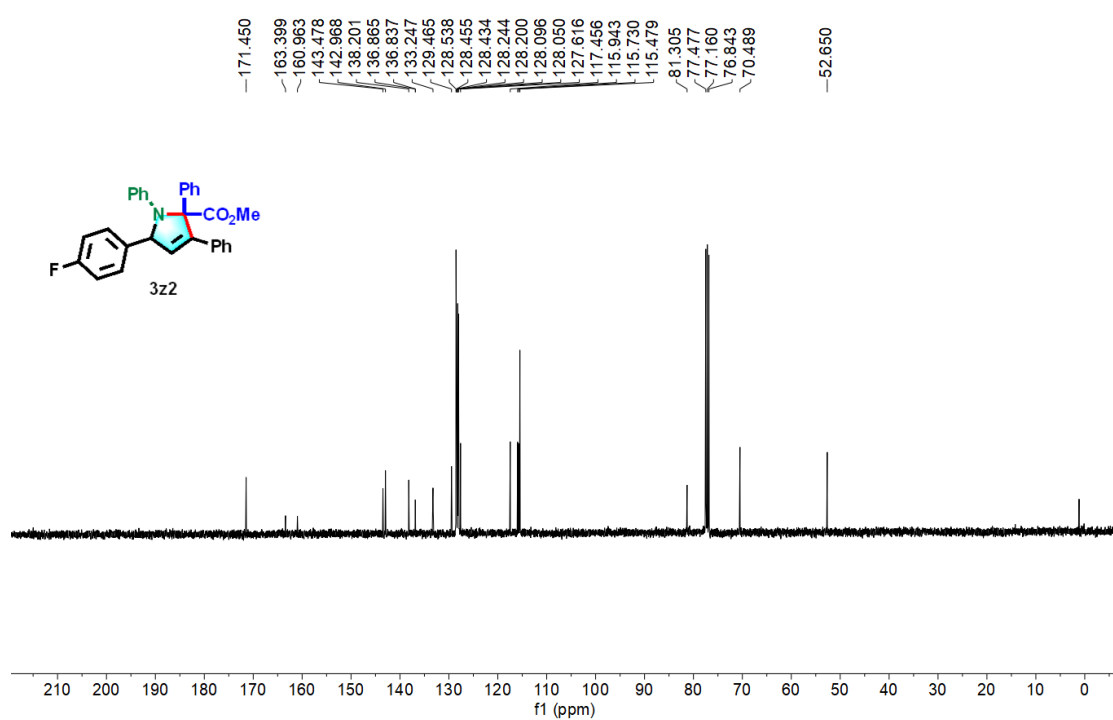
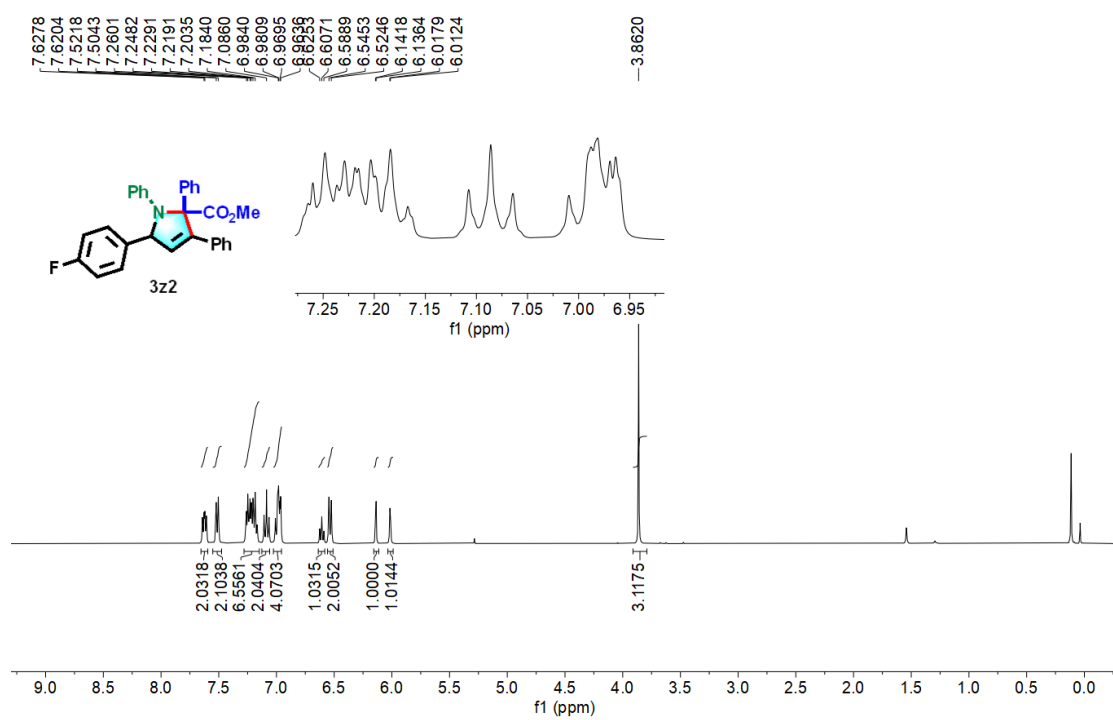




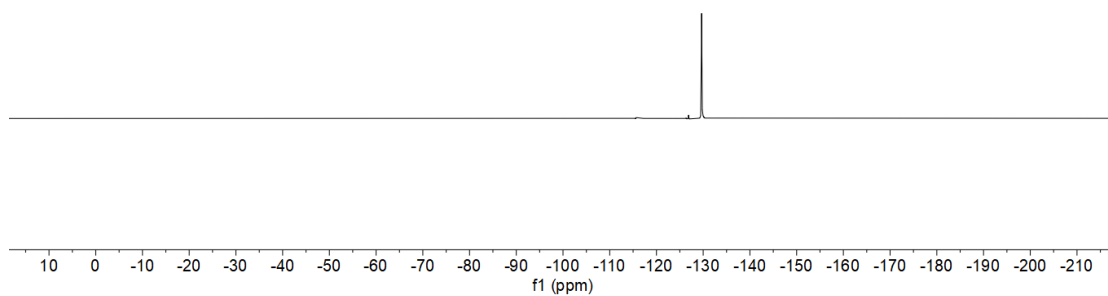
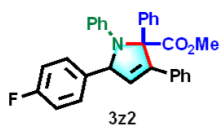




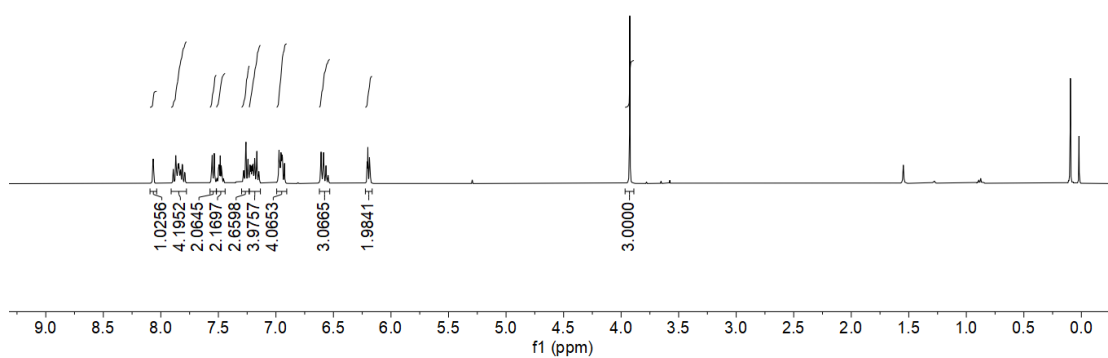
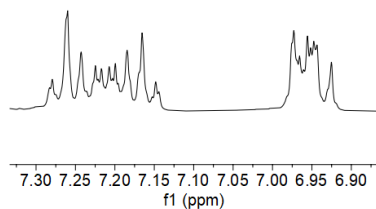
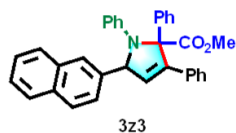


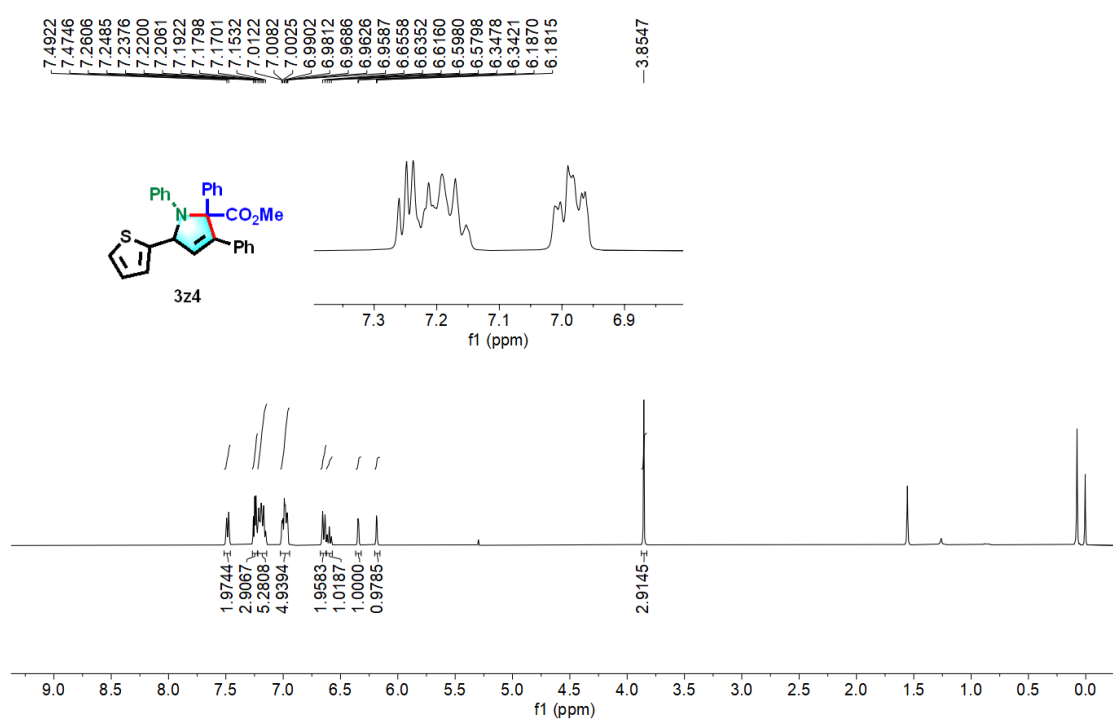
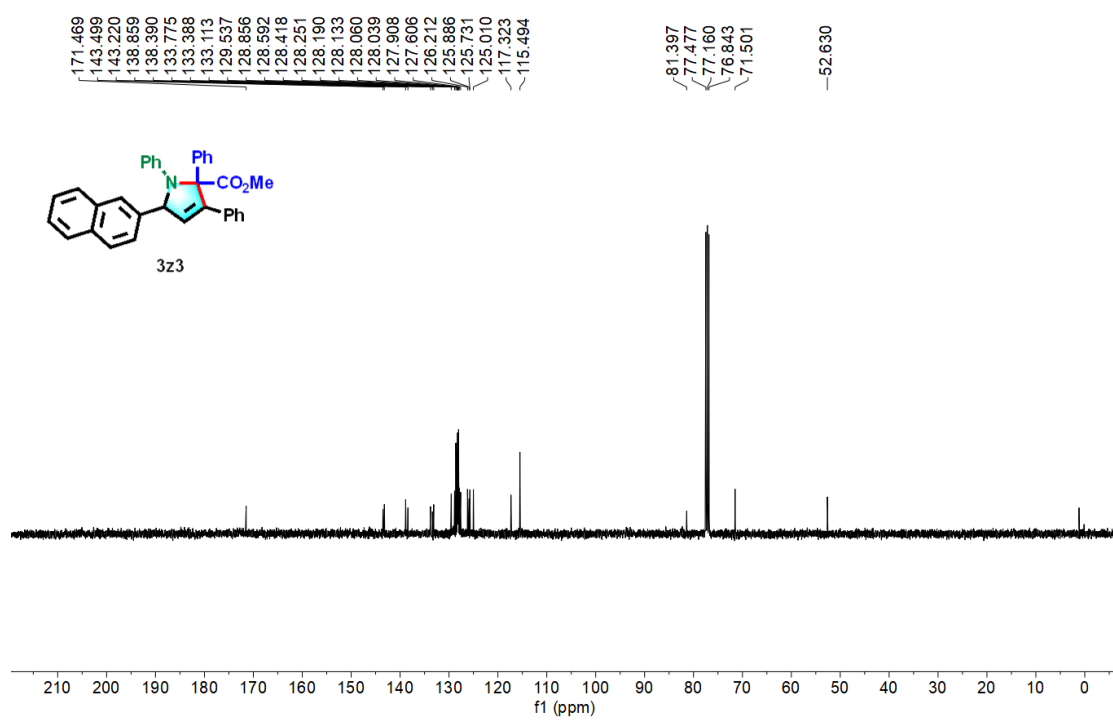


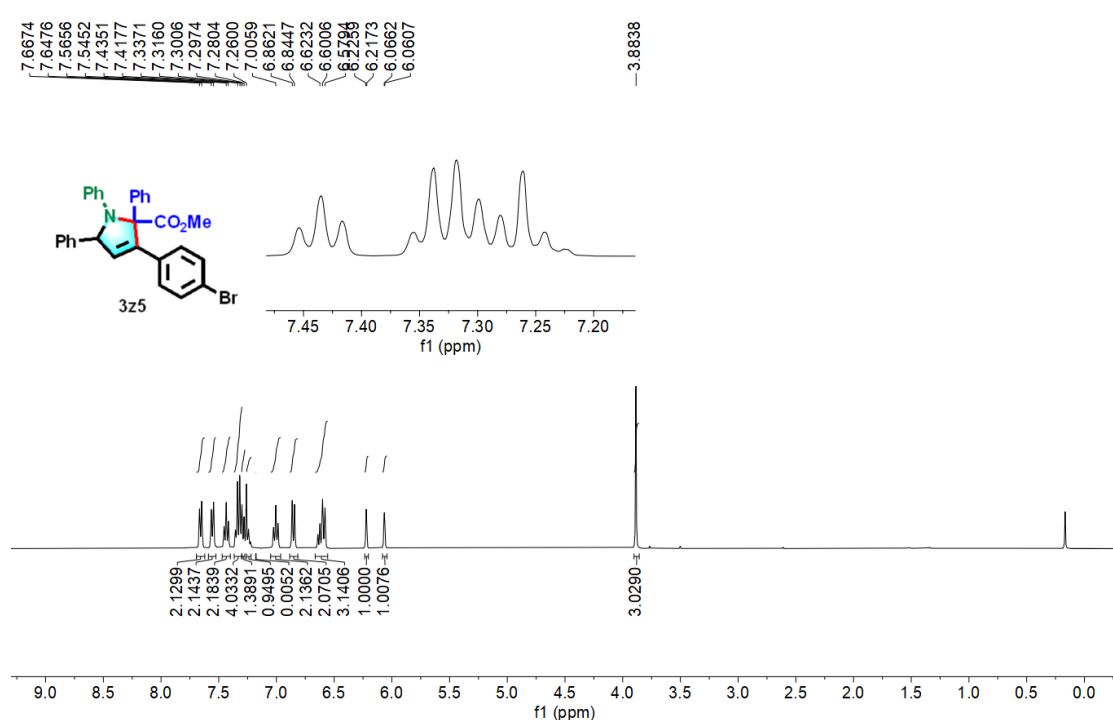
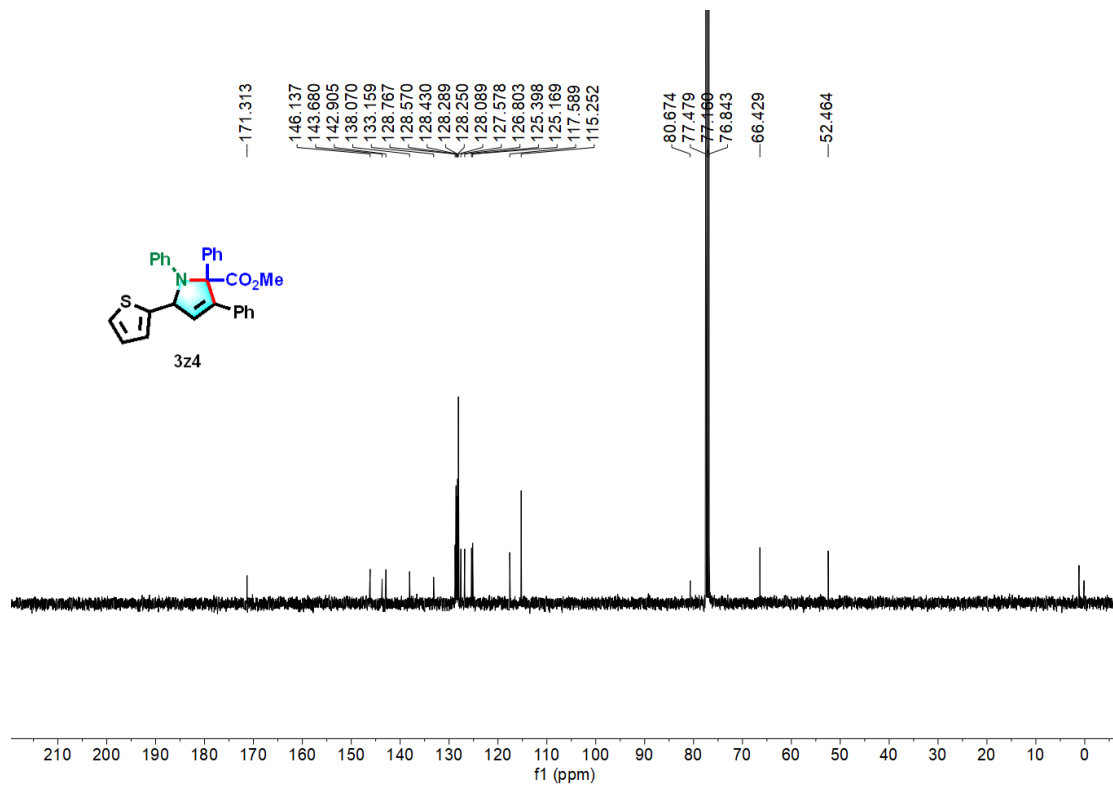
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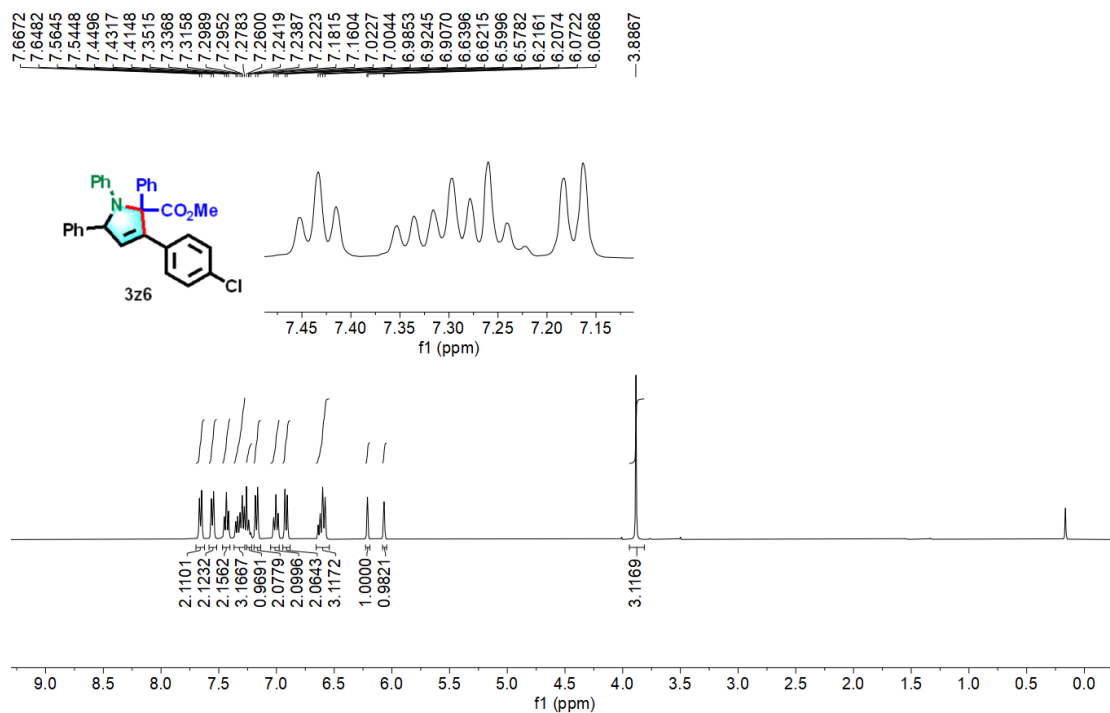
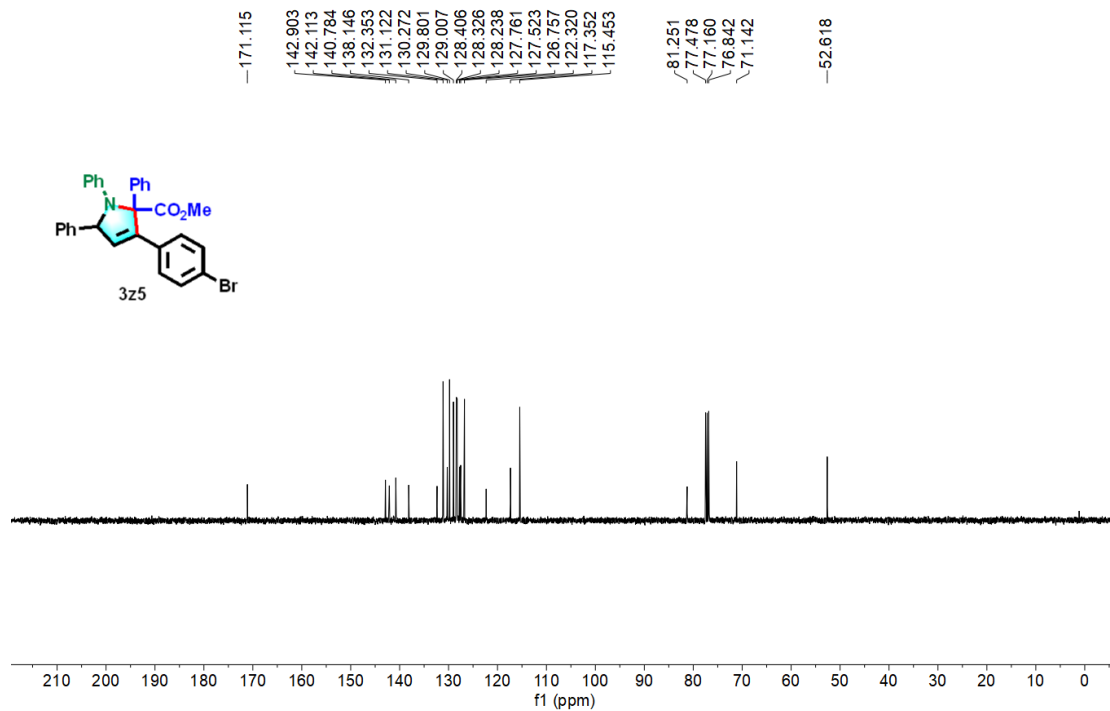


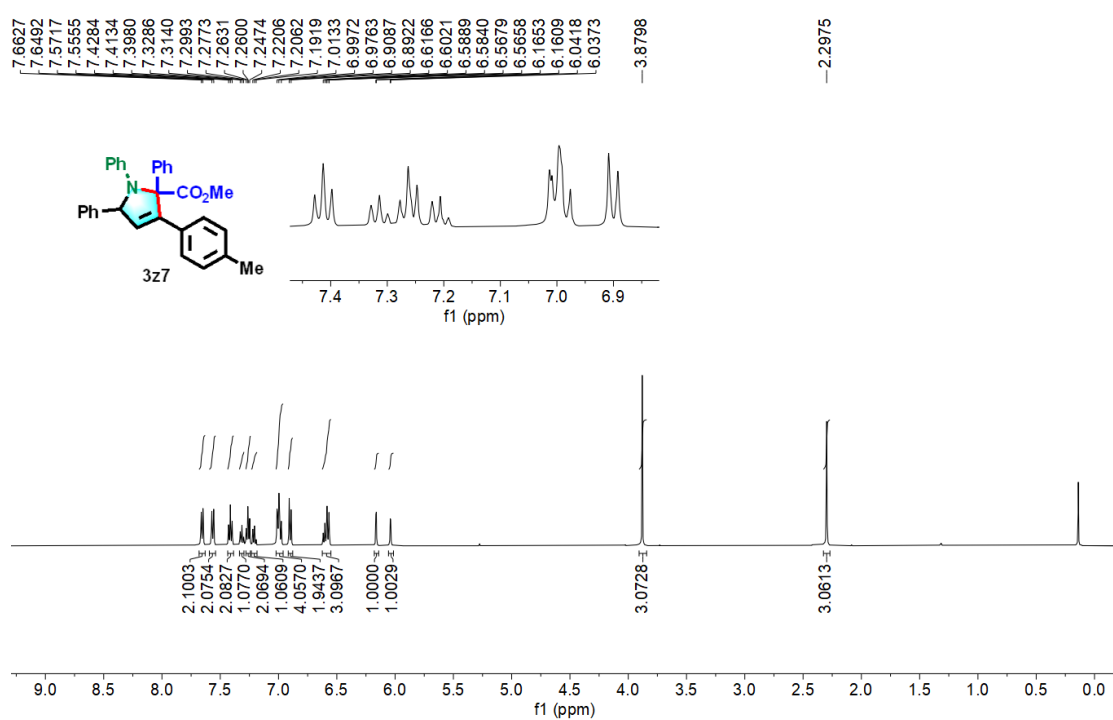
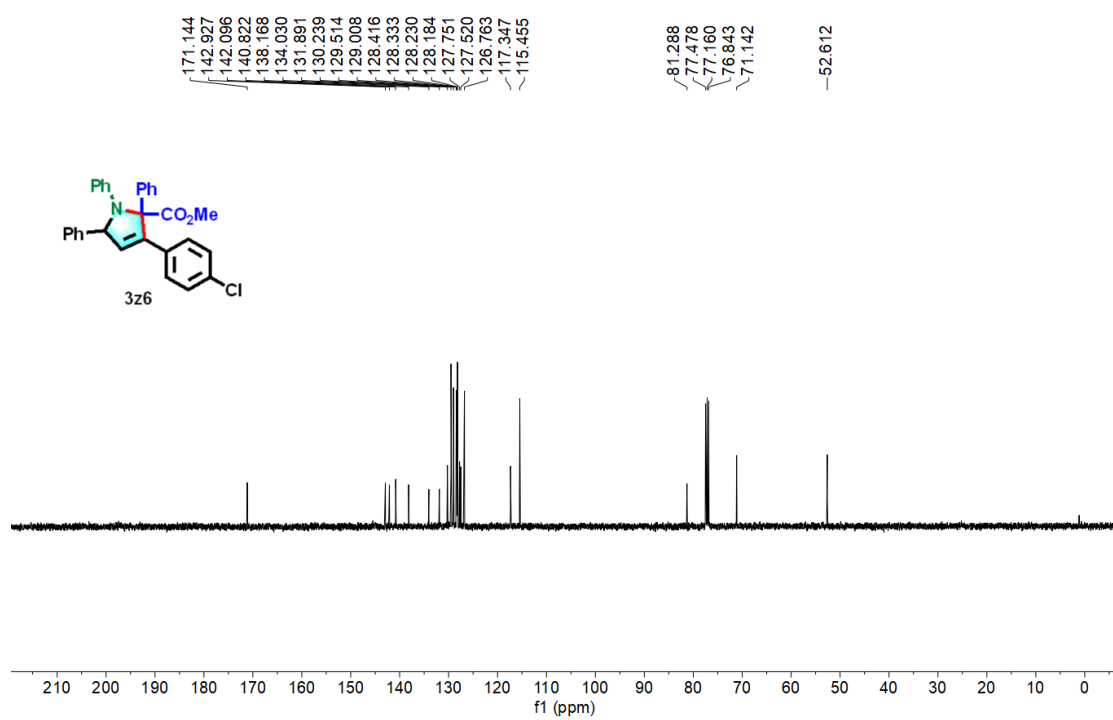
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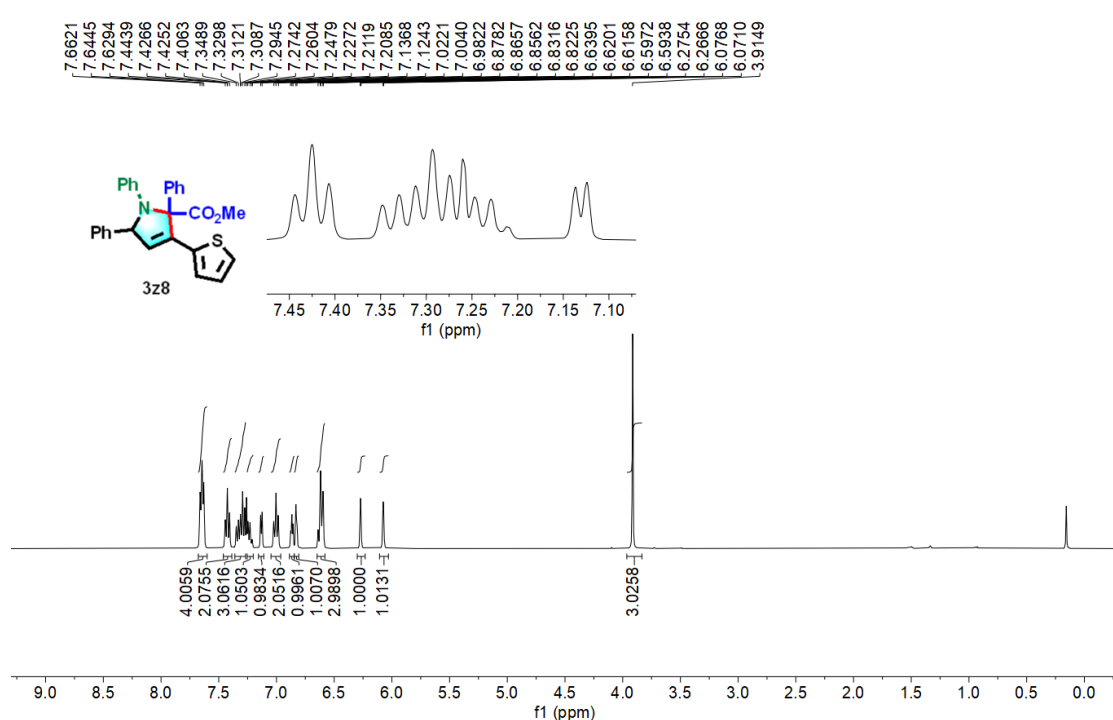
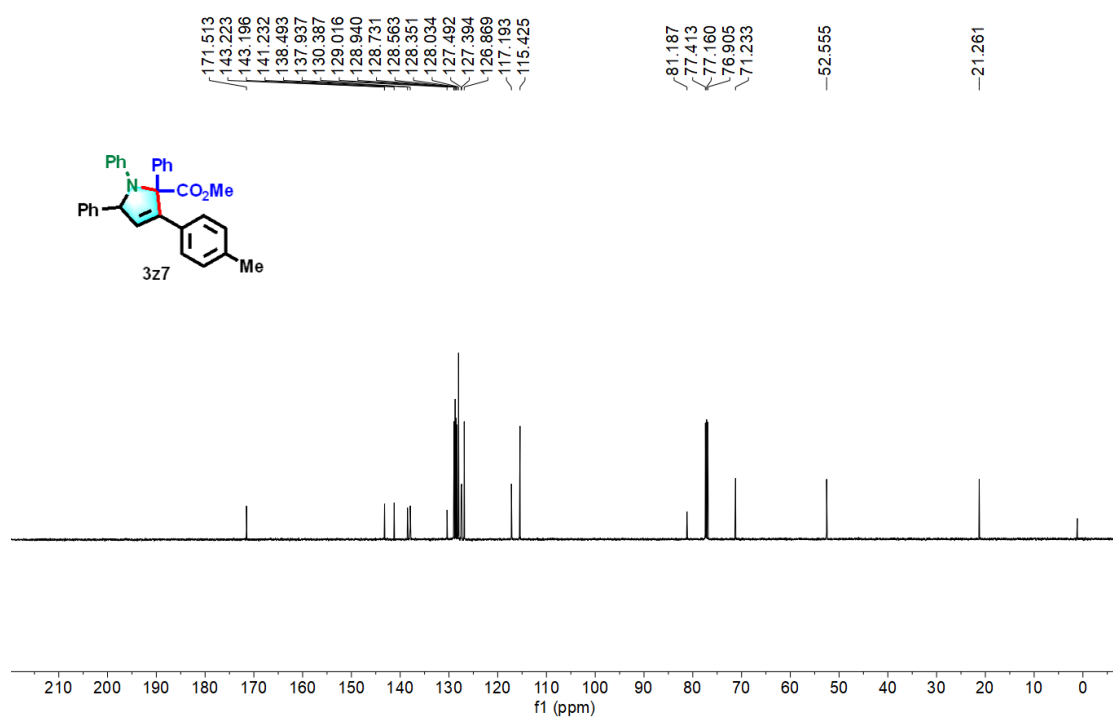




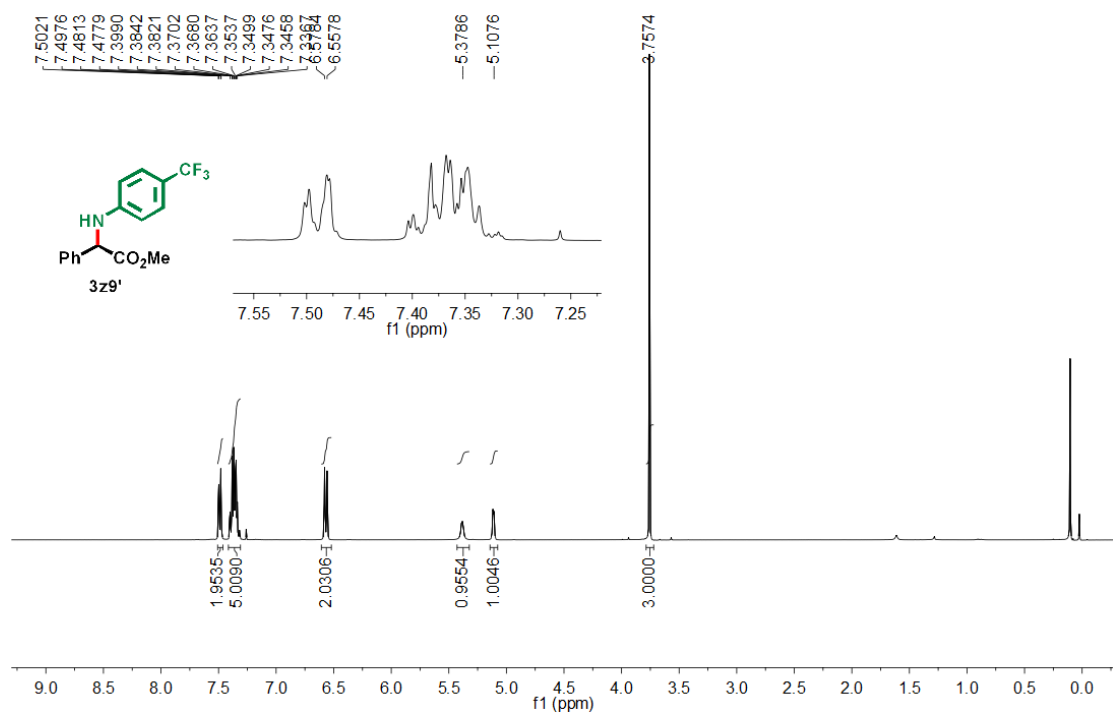
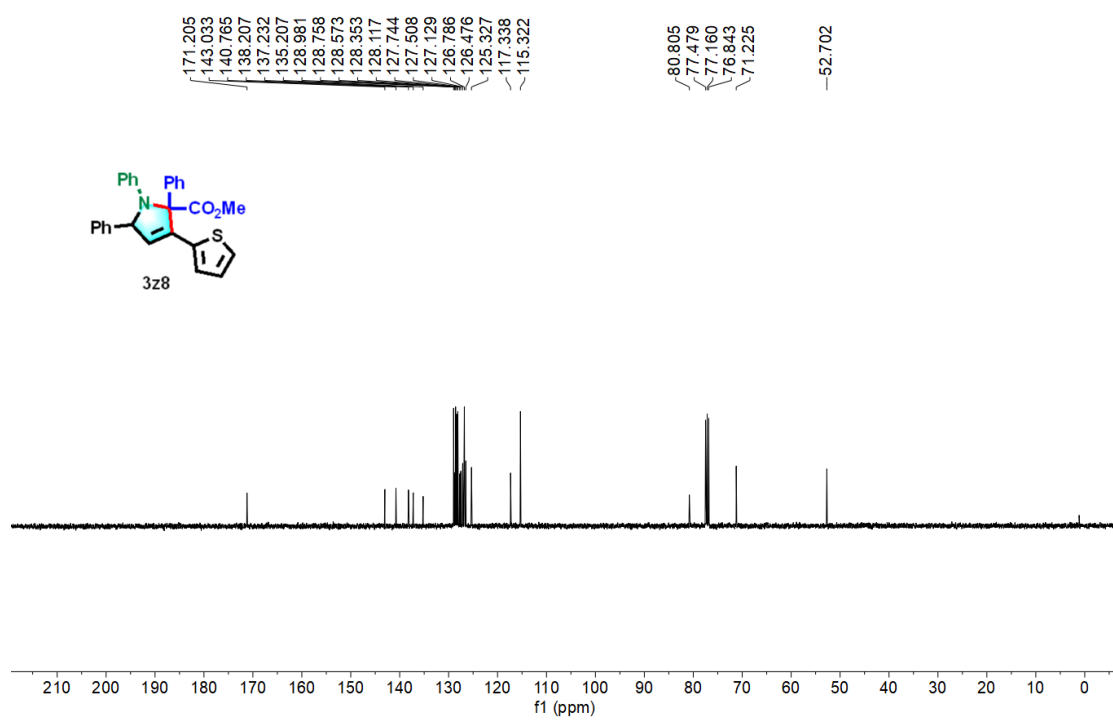


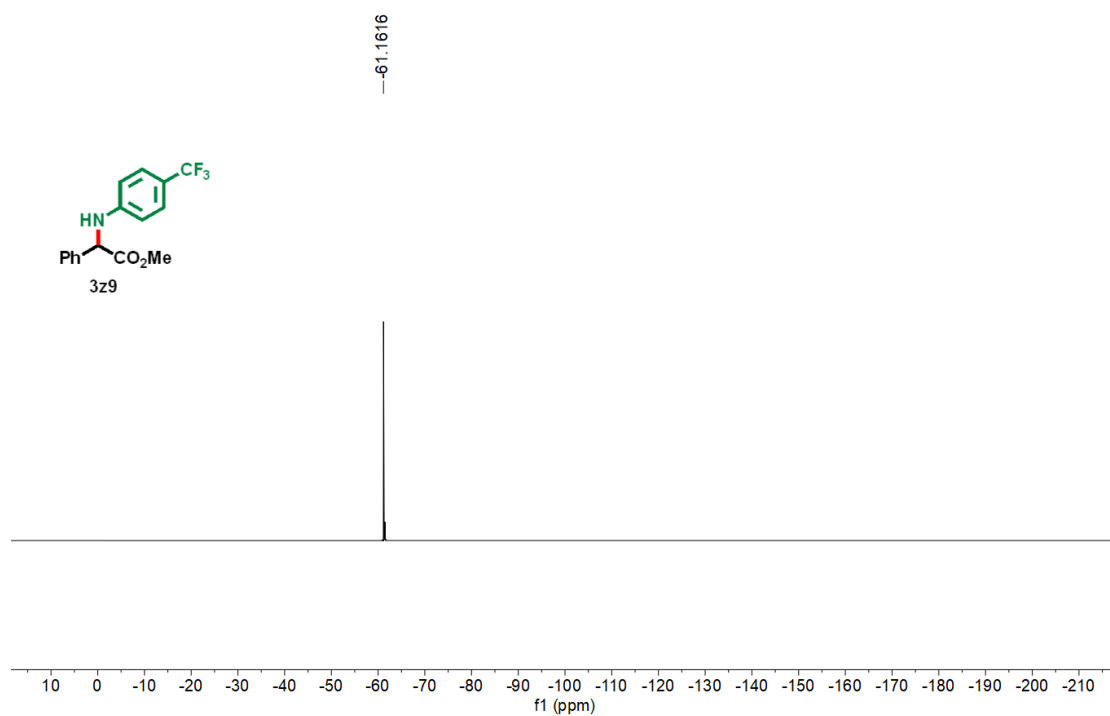
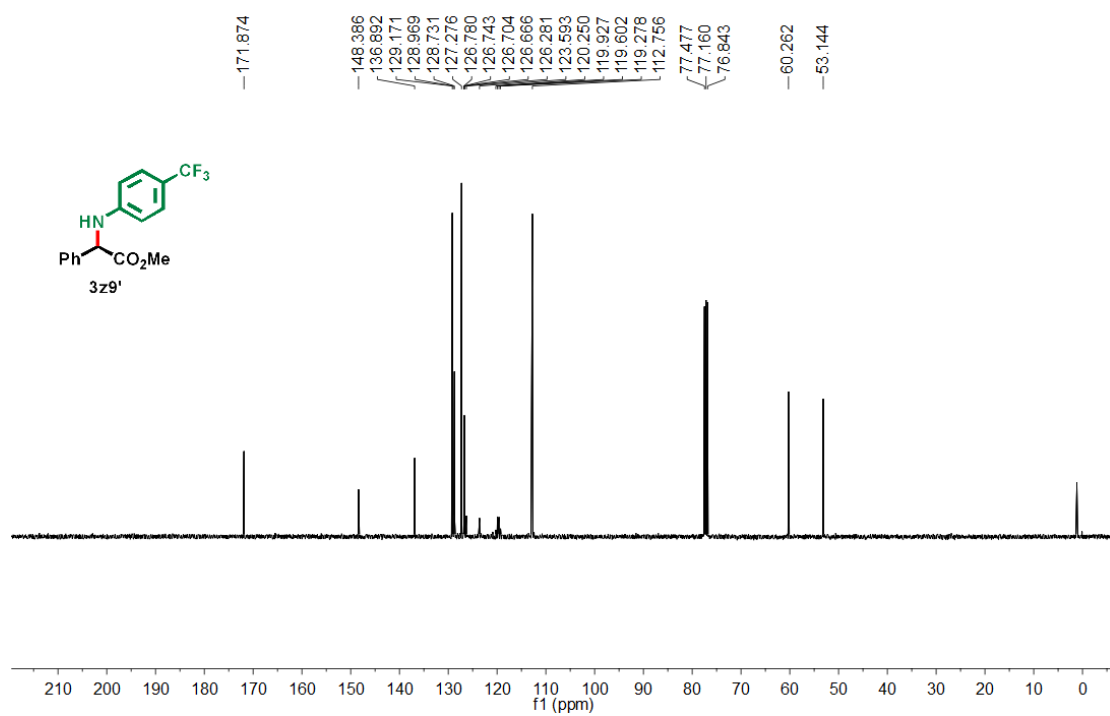


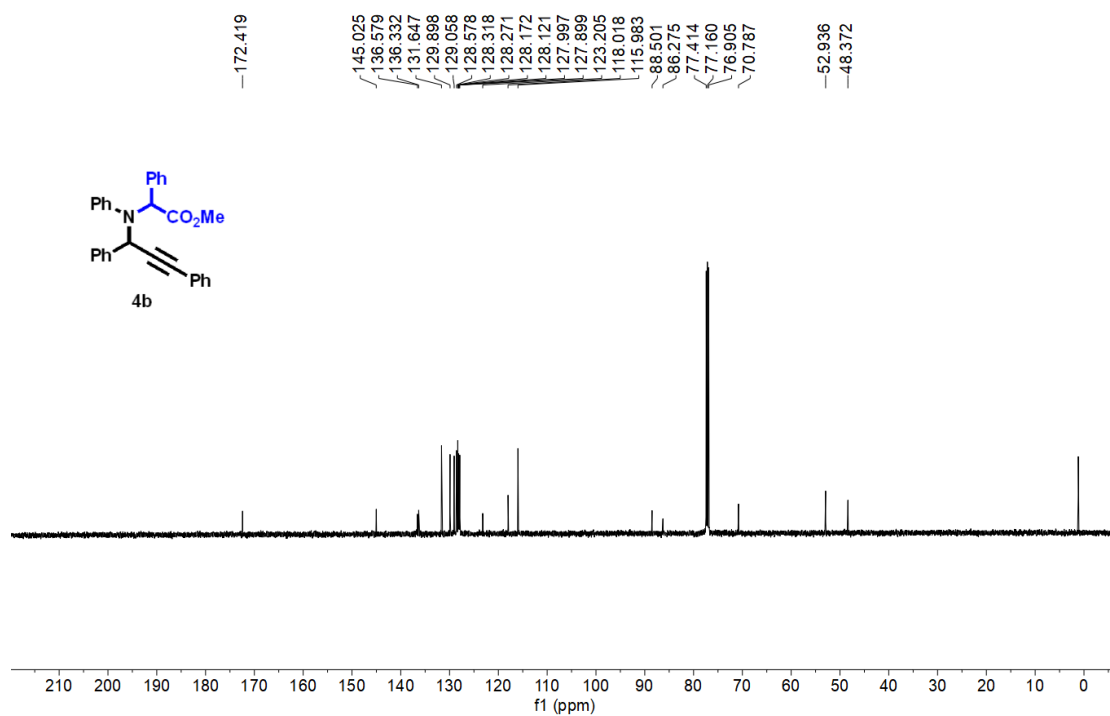
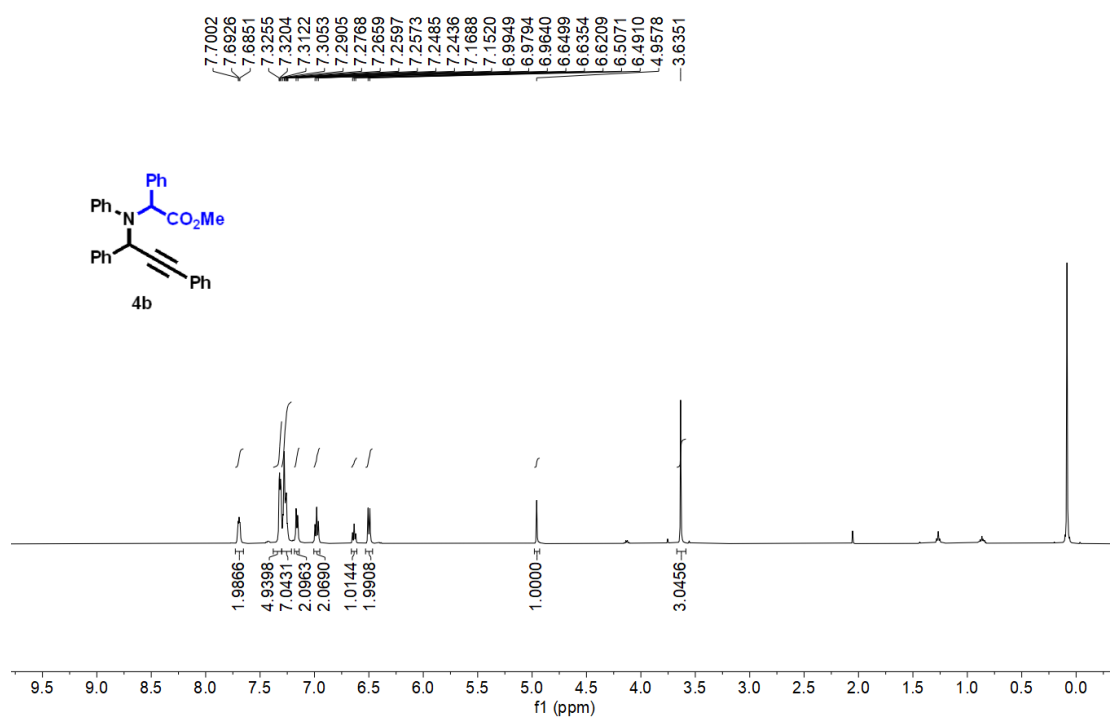


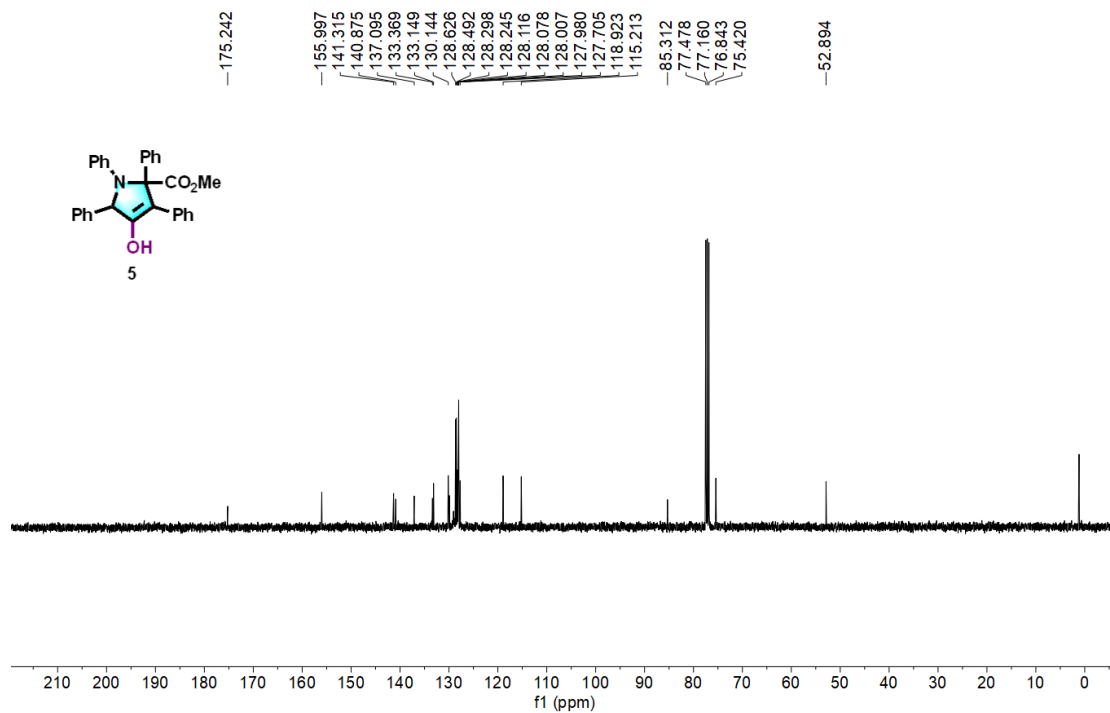
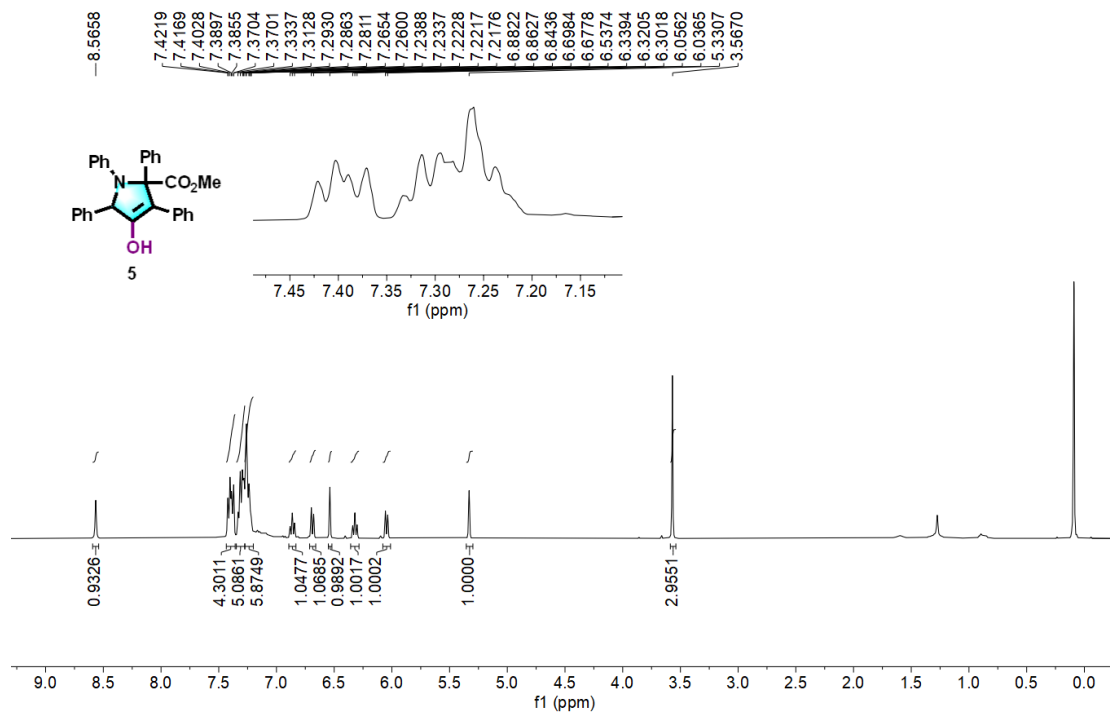


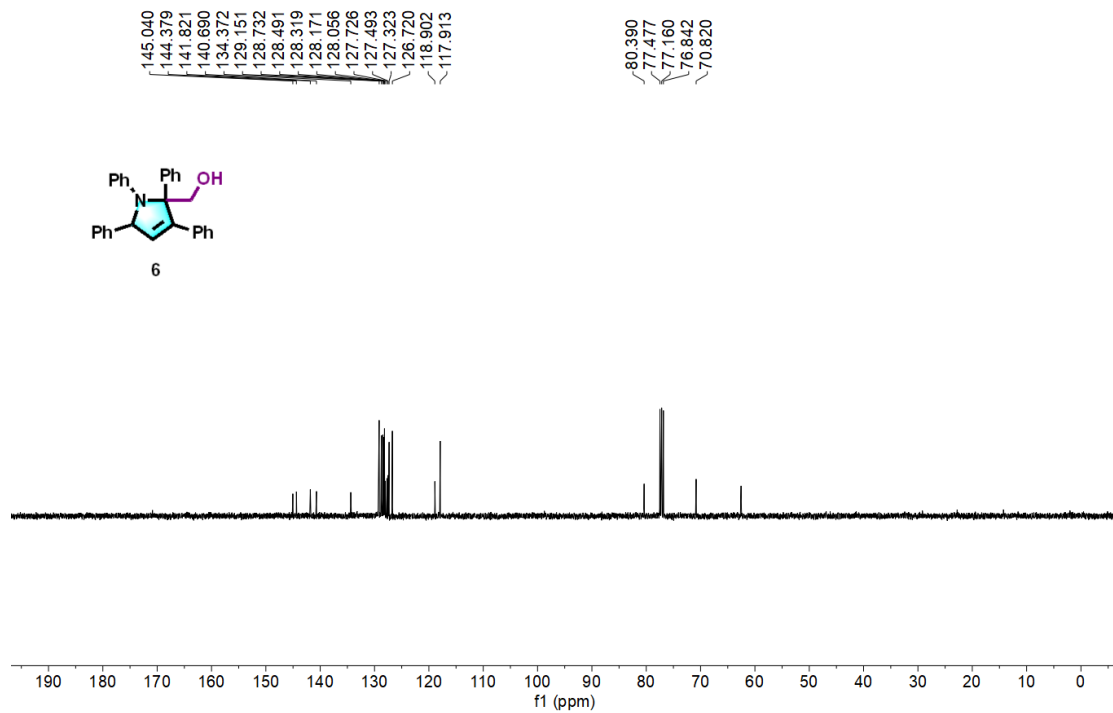
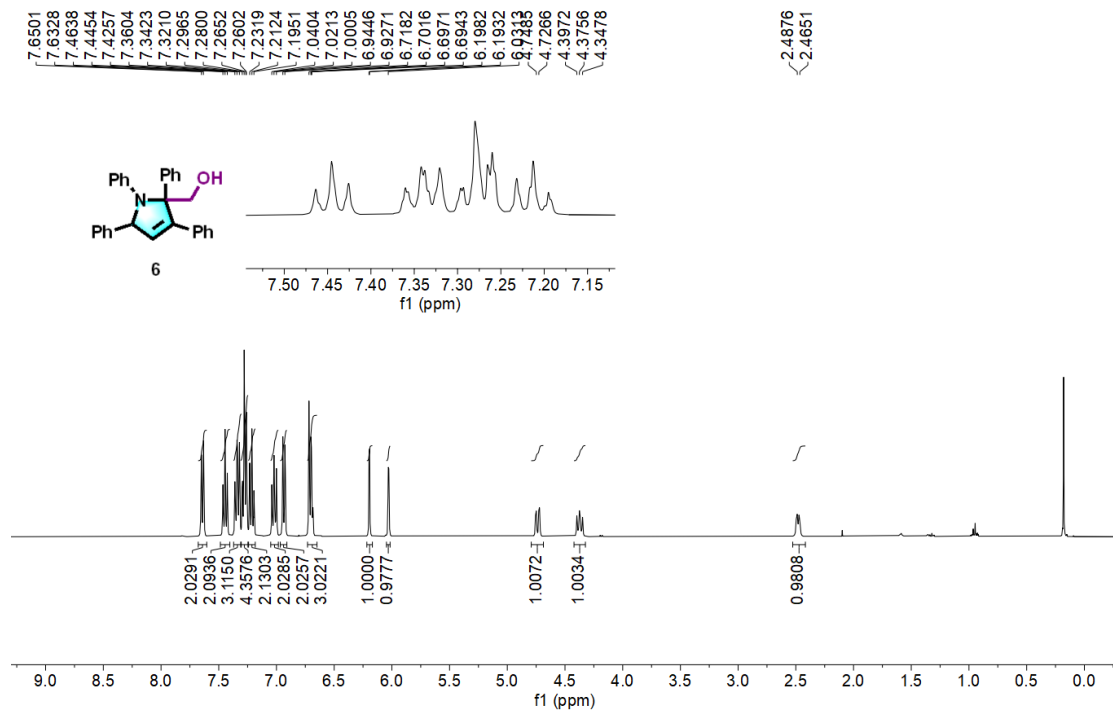












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