Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Gold-catalyzed cascade C–H/C–H cross-coupling/cyclization/alkynylation: An efficient access to 3-alkynylpyrroles

Shuai Zhang, Yuanhong Ma, Jingbo Lan, Feijie Song* and Jingsong You*

Key Laboratory of Green Chemistry and Technology of Ministry of Education, College of Chemistry, and State Key Laboratory of Biotherapy, West China Medical School, Sichuan University, 29 Wangjiang Road, Chengdu 610064, PR China

Fax: 86-28-85412203; E-mail: jsyou@scu.edu.cn; fsong@scu.edu.cn

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I. General remarks

NMR spectra were obtained on a Bruker AV II-400 MHz (^{1}H NMR at 400 MHz, ^{13}C NMR at 100 MHz, and ^{19}F NMR at 376 MHz). The ^{1}H NMR chemical shifts were measured relative to $CDCl_3$ (δ = 7.26 ppm) or DMSO-d_6 (δ = 2.50 ppm) as the internal reference. The ^{13}C NMR chemical shifts were given using $CDCl_3$ (δ = 77.16 ppm) or DMSO-d_6 (δ = 39.52 ppm) as the internal standard. High-resolution mass spectra (HRMS) were obtained with a Waters-Q-TOF-Premier (ESI). X-Ray single-crystal diffraction data were collected on an Oxford Xcalibur E or Agilent Technologies Gemini single crystal diffractometers. Melting points were determined with XRC-1 and are uncorrected.

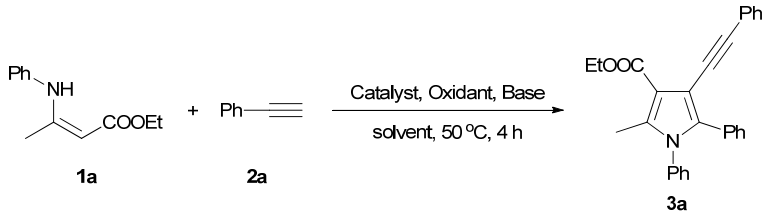
Unless otherwise noted, all reactions were carried out under N_2. All reagents were obtained from commercial suppliers and used without further purification. $HAuCl_4 \cdot xH_2O$ (≥ 50% Au) were purchased from Shanxi Kaida Chemical Engineering (China) Co., Ltd. $AuCl_3$ and $AuBr_3$ were purchased from Acros and Alfa Aesar, respectively. [(bpy)$AuCl_2$]Cl,[1] 1-ethynyl-2-(methoxymethoxy)benzene,[2] 4-ethynylbenzonitrile,[3] 1-ethynylnaphthalene,[4] 2-ethynylthiophene,[5] *β*-aryl enamines **1h-1l**,[6a] *β*-alkyl enamines **1a-1g** and **1m-1p**,[6b] and α,*β*-disubstituted enamines **1q-1r**[6c] were prepared according to the literature procedure. Solvents were dried by refluxing over CaH_2 (for CH_2Cl_2, DMF, CH_3CN, and PhCl) or sodium (for toluene, THF, and MeOH) and freshly distilled prior to use.

II. Optimization of the reaction of *β*-enamino esters with terminal alkynes

A flame-dried sealable tube with a magnetic stir bar was charged with gold species, base, oxidant, (*Z*)-ethyl 3-(phenylamino)but-2-enoate **1a** (232.4 μL, 1.2 mmol), phenylacetylene **2a** (65.9 μL, 0.6 mmol), and solvent (3.0 mL) under an N_2 atmosphere. The tube was sealed and the reaction mixture was stirred at 50 °C for 4 h. After being cooled to ambient temperature, the reaction solution was diluted with 10 mL of CH_2Cl_2, filtered through a celite pad, and washed with 30 mL of CH_2Cl_2. The filtrate was concentrated and the residue was purified by column chromatography on

silica gel (petroleum ether/ethyl acetate = 20/1, v/v) to provide the desired product **3a**.

Table S1. Optimization of the gold-catalyzed reaction of (*Z*)-ethyl 3-(phenylamino)but-2-enoate **1a** with phenylacetylene **2a**[a]



entry	catalyst (mol%)	oxidant	base (equiv)	solvent	yield (%)
1	none	$PhI(OAc)_2$	KOAc (2.0)	toluene	0
2	Ph_3PAuCl (4)	$PhI(OAc)_2$	KOAc (2.0)	toluene	45
3	$AuCl_3$ (4)	$PhI(OAc)_2$	KOAc (2.0)	toluene	42
4	$AuBr_3$ (4)	$PhI(OAc)_2$	KOAc (2.0)	toluene	34
5	$HAuCl_4{\cdot}xH_2O$ (4)	$PhI(OAc)_2$	KOAc (2.0)	toluene	30
6	$AuCl_3$ (4) + bpy (4)	$PhI(OAc)_2$	KOAc (2.0)	toluene	42
7	$AuCl_3$ (4) + phen (4)	$PhI(OAc)_2$	KOAc (2.0)	toluene	26
8	$[(bpy)AuCl_2]Cl$ (4)	$PhI(OAc)_2$	KOAc (2.0)	toluene	57
9	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	KOAc (2.0)	toluene	61
10	$[(bpy)AuCl_2]Cl$ (10)	$PhI(OAc)_2$	KOAc (2.0)	toluene	54
11	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OPiv)_2$	KOAc (2.0)	toluene	38
12	$[(bpy)AuCl_2]Cl$ (5)	PIFA	KOAc (2.0)	toluene	0
13	$[(bpy)AuCl_2]Cl$ (5)	$K_2S_2O_8$	KOAc (2.0)	toluene	0
14	$[(bpy)AuCl_2]Cl$ (5)	NFSI	KOAc (2.0)	toluene	0
15	$[(bpy)AuCl_2]Cl$ (5)	Selectfluor	KOAc (2.0)	toluene	0
16	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	KOAc (2.0)	DCM	43
17	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	KOAc (2.0)	PhCl	44
18	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	KOAc (2.0)	THF	21
19	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	KOAc (2.0)	CH_3CN	trace
20	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	KOAc (2.0)	DMF	0
21	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	KOAc (2.0)	MeOH	0
22	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	none	toluene	39
23	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	NaOAc (2.0)	toluene	40
24	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	CsOAc (2.0)	toluene	52
25	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	K_3PO_4 (2.0)	toluene	44
26	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	Cs_2CO_3 (2.0)	toluene	50
27	$[(bpy)AuCl_2]Cl$ (5)	$PhI(OAc)_2$	KOAc (3.0)	toluene	66
28	$[(bpy)AuCl_2]Cl$ (4)	$PhI(OAc)_2$	KOAc (3.0)	toluene	60

29[b]	[(bpy)$AuCl_2$]Cl (4)	$PhI(OAc)_2$	KOAc (3.0)	toluene	35
30[c]	**[(bpy)$AuCl_2$]Cl (4)**	**$PhI(OAc)_2$**	**KOAc (3.0)**	**toluene**	**66**

[a] Reaction conditions: **1a** (1.2 mmol), **2a** (0.6 mmol), gold species, base (2.0-3.0 equiv), oxidant (2.0 equiv), and solvent (3.0 mL) at 50 °C for 4 h. Isolated yields based on **2a** are given. [b] The ratio of **1a/2a** was 1/1. [c] The ratio of **1a/2a** was 2.5/1. bpy = 1,2-bipyridine; PIFA = phenyliodine bis(trifluoroacetate); NFSI = *N*-fluorobenzenesulfonimide; Selectfluor = 1-chloromethyl-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane bis(tetrafluoroborate).

III. General procedure for the synthesis of fully substituted 3-alykynlpyrroles

A flame-dried sealable tube with a magnetic stir bar was charged with [(bpy)$AuCl_2$]Cl (11.1 mg, 0.024 mmol), KOAc (176.7 mg, 1.8 mmol), $PhI(OAc)_2$ (386.5 mg, 1.2 mmol), *β*-enamino ester **1** (1.5 mmol), terminal alkyne **2** (0.6 mmol), and toluene (3.0 mL) under an N_2 atmosphere. The tube was sealed and the reaction mixture was stirred at 50 °C for 4 h. After being cooled to ambient temperature, the reaction solution was diluted with 10 mL of CH_2Cl_2, filtered through a celite pad, and washed with 30 mL of CH_2Cl_2. The filtrate was evaporated and the residue was purified by column chromatography on silica gel to provide the desired product **3** and **4**.

IV. General procedure for the synthesis of C5-unsubstituted 3-alkynylpyrroles

A flame-dried sealable tube with a magnetic stir bar was charged with [(bpy)$AuCl_2$]Cl (9.2 mg, 0.02 mmol), KOAc (117.8 mg, 1.2 mmol), $PhI(OAc)_2$ (257.7 mg, 0.8 mmol), 2,3-disubstituted *β*-enamino ester **1** (1.2 mmol), terminal alkyne **2** (0.4 mmol), and chlorobenzene (2.0 mL) under an N_2 atmosphere. The tube was sealed and the reaction mixture was stirred at 50 °C for 4 h. After being cooled to ambient temperature, chlorobenzene was evaporated and the residue was diluted with 10 mL of CH_2Cl_2, filtered through a celite pad, and washed with 30 mL of CH_2Cl_2. The filtrate was concentrated and the residue was purified by column chromatography on silica gel to provide the desired product **5**.

V. ORTEP diagrams of compounds 3a and 11a

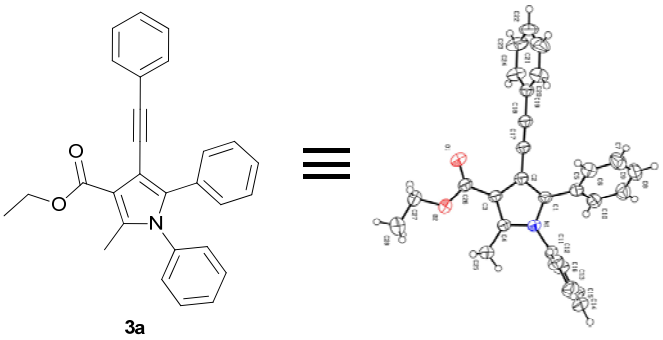


Figure S1. ORTEP diagram of **3a** (CCDC 1031864). Thermal ellipsoids are set at 50% probability.

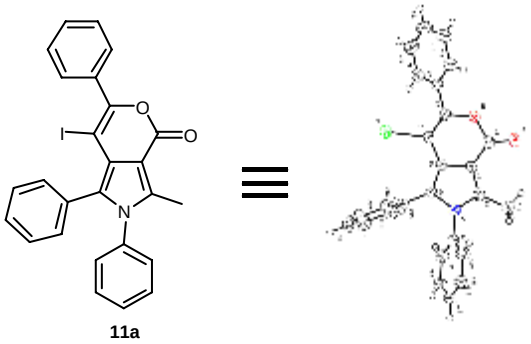
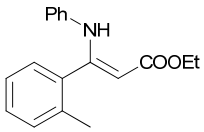


Figure S2. ORTEP diagram of **11a** (CCDC 1031865). Thermal ellipsoids are set at 50% probability.

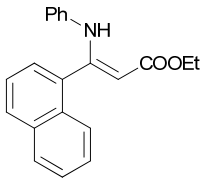
VI. Characterization of new *β*-enamino esters



(*Z*)-Ethyl 3-(phenylamino)-3-(*o*-tolyl)acrylate (1i)[6a]

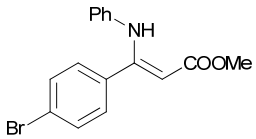
Purification by column chromatography on basic Al_2O_3 (petroleum ether/ethyl acetate = 20/1, v/v) afforded **1i** as a pale yellow solid in 49% yield. M.p.: 84-86 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.32 (t, J = 7.2 Hz, 3H), 2.12 (s, 3H), 4.22 (q, J = 7.2 Hz, 2H), 4.76 (s, 1H), 6.58 (d, J = 7.6 Hz, 2H), 6.88 (t, J = 7.6 Hz, 1H), 7.03 (t, J = 7.6 Hz, 2H), 7.08 (d, J = 7.6 Hz, 1H), 7.21 (t, J = 7.6 Hz, 1H), 7.27 (td, J = 7.6 Hz, 1.6 Hz, 1H), 7.32 (dd, J = 7.6 Hz, 1.6 Hz, 1H), 10.62 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ

= 14.7, 19.6, 59.3, 89.6, 120.8, 123.1, 126.1, 128.8, 129.0, 129.3, 130.4, 135.7, 136.0, 140.0, 159.5, 170.4 ppm. HRMS (ESI^+): calcd for $C_{18}H_{19}NNaO_2$ $[M+Na]^+$ 304.1313, found 304.1318.



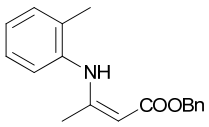
(*Z*)-Ethyl 3-(naphthalen-1-yl)-3-(phenylamino)acrylate (1j)[6a]

Purification by column chromatography on basic Al_2O_3 (petroleum ether/ethyl acetate = 20/1, v/v) afforded **1j** as a white solid in 30% yield. M.p.: 108-110 ºC. ^1H NMR ($CDCl_3$, 400 MHz): δ = 1.34 (t, J = 7.2 Hz, 3H), 4.25 (q, J = 6.8 Hz, 2H), 4.95 (s, 1H), 6.55 (d, J = 8.0 Hz, 2H), 6.76 (t, J = 7.6 Hz, 1H), 6.89 (t, J = 8.0 Hz, 2H), 7.41-7.47 (m, 4H), 7.80-7.86 (m, 2H), 8.09-8.12 (m, 1H), 10.81 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 14.7, 59.4, 91.2, 121.2, 123.2, 125.2, 125.4, 126.3, 126.9, 127.0, 128.4, 128.7, 129.6, 130.7, 133.5, 133.9, 140.0, 158.3, 170.4 ppm. HRMS (ESI^+): calcd for $C_{21}H_{19}NNaO_2$ $[M+Na]^+$ 340.1313, found 340.1315.



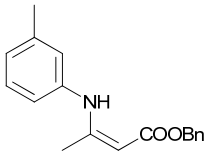
(*Z*)-Methyl 3-(4-bromophenyl)-3-(phenylamino)acrylate (1l)[6a]

Purification by column chromatography on basic Al_2O_3 (petroleum ether/ethyl acetate = 20/1, v/v) afforded **1l** as a white solid in 48% yield. M.p.: 88-90 ºC. ^1H NMR ($CDCl_3$, 400 MHz): δ = 3.74 (s, 3H), 4.98 (s, 1H), 6.67 (d, J = 7.6 Hz, 2H), 6.94 (t, J = 7.2 Hz, 1H), 7.11 (t, J = 8.0 Hz, 2H), 7.21 (dt, J = 8.8 Hz, 2.0 Hz, 2H), 7.42 (dt, J = 8.8 Hz, 2.0 Hz, 2H), 10.22 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 50.9, 91.1, 122.6, 123.5, 123.9, 128.9, 129.9, 131.8, 135.0, 140.2, 158.0, 170.4 ppm. HRMS (ESI^+): calcd for $C_{16}H_{14}BrNNaO_2$ $[M+Na]^+$ 354.0106, found 354.0109.



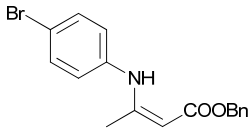
(*Z*)-Benzyl 3-(*o*-tolylamino)but-2-enoate (1m)[6b]

Purification by column chromatography on basic Al_2O_3 (petroleum ether/ethyl acetate = 20/1, v/v) afforded **1m** as colorless oil in 89% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.86 (s, 3H), 2.30 (s, 3H), 4.78 (s, 1H), 5.17 (s, 2H), 7.08 (dd, J = 7.2 Hz, 1.2 Hz, 1H), 7.12-7.20 (m, 2H), 7.22-7.24 (m, 1H), 7.29-7.33 (m, 1H), 7.35-7.42 (m, 4H), 10.12 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 18.2, 20.3, 64.8, 85.0, 126.3, 126.6, 126.7, 128.0, 128.1, 128.6, 130.9, 134.1, 137.4, 138.0, 160.5, 170.4 ppm. HRMS (ESI$^+$): calcd for $C_{18}H_{19}NNaO_2$ $[M+Na]^+$ 304.1313, found 304.1316.



(*Z*)-Benzyl 3-(*m*-tolylamino)but-2-enoate (**1n**)[6b]

Purification by column chromatography on basic Al_2O_3 (petroleum ether/ethyl acetate = 20/1, v/v) afforded **1n** as a pale brown solid in 58% yield. M.p.: 50-52 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.01 (s, 3H), 2.35 (s, 3H), 4.77 (s, 1H), 5.17 (s, 2H), 6.90-6.92 (m, 2H), 6.99 (d, J = 6.8 Hz, 1H), 7.20-7.23 (m, 1H), 7.29-7.40 (m, 5H), 10.35 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.5, 21.5, 64.7, 85.5, 121.7, 125.4, 126.0, 127.9, 128.0, 128.6, 128.9, 137.3, 139.1, 139.2, 159.7, 170.2 ppm. HRMS (ESI$^+$): calcd for $C_{18}H_{19}NNaO_2$ $[M+Na]^+$ 304.1313, found 304.1311.

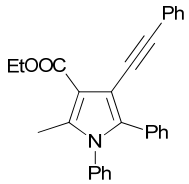


(*Z*)-Benzyl 3-((4-bromophenyl)amino)but-2-enoate (1o)[6b]

Purification by column chromatography on basic Al_2O_3 (petroleum ether/ethyl acetate = 20/1, v/v) afforded **1o** as a white solid in 55% yield. M.p.: 58-60 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.99 (s, 3H), 4.80 (s, 1H), 5.16 (s, 2H), 6.96 (d, J = 8.8 Hz,

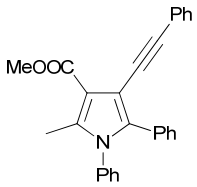
2H), 7.31-7.40 (m, 5H), 7.43-7.45 (m, 2H), 10.33 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.4, 64.9, 86.8, 118.3, 126.0, 128.0, 128.6, 132.3, 137.1, 138.5, 158.9, 170.1 ppm. HRMS (ESI^+): calcd for $C_{17}H_{16}BrNNaO_2$ $[M+Na]^+$ 368.0262, found 368.0261.

VII. Characterization of products 3-5



Ethyl 2-methyl-1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3a)

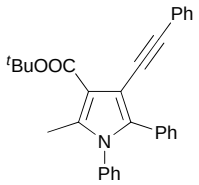
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3a** as a pale yellow solid (80.2 mg, 66% yield). M.p.: 140-142 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.45 (t, J = 7.2 Hz, 3H), 2.41 (s, 3H), 4.41 (q, J = 7.2 Hz, 2H), 7.10-7.12 (m, 2H), 7.18-7.22 (m, 3H), 7.26-7.30 (m, 5H), 7.36-7.40 (m, 5H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 12.9, 14.7, 60.0, 85.2, 91.5, 104.4, 113.5, 124.7, 127.41, 127.44, 127.8, 128.2, 128.55, 128.63, 129.3, 130.1, 130.8, 131.2, 137.6, 137.9, 138.1, 165.2 ppm. HRMS (ESI^+): calcd for $C_{28}H_{23}NNaO_2$ $[M+Na]^+$ 428.1626, found 428.1627.



Methyl 2-methyl-1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3b)

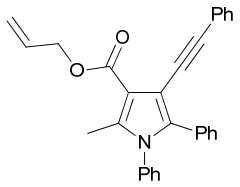
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3b** as a pale yellow solid (80.8 mg, 69% yield). M.p.: 158-160 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.40 (s, 3H), 3.94 (s, 3H), 7.09-7.11 (m, 2H), 7.16-7.22 (m, 3H), 7.23-7.30 (m, 5H), 7.33-7.37 (m, 3H), 7.39 (dd, J = 7.6 Hz, 1.2 Hz , 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 12.9, 51.2, 85.1, 91.7, 104.5, 113.5, 124.6, 127.4, 127.5, 127.8, 128.2, 128.59, 128.63, 129.3, 130.1, 130.8, 131.3, 137.6, 138.01,

138.05, 165.6 ppm. HRMS (ESI^+): calcd for $C_{27}H_{21}NNaO_2$ $[M+Na]^+$ 414.1470, found 414.1478.



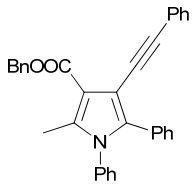
***tert*-Butyl 2-methyl-1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3c)**

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3c** as a pale yellow solid (85.3 mg, 66% yield). M.p.: 182-184 ºC. ^1H NMR ($CDCl_3$, 400 MHz): δ = 1.64 (s, 9H), 2.39 (s, 3H), 7.08-7.11 (m, 2H), 7.16-7.21 (m, 3H), 7.23-7.30 (m, 5H), 7.34-7.39 (m, 5H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 12.8, 28.8, 80.4, 85.6, 91.2, 104.3, 114.7, 124.8, 127.3, 127.4, 127.7, 128.2, 128.5, 128.6, 129.3, 130.1, 130.9, 131.3, 137.4, 137.7, 138.1, 164.5 ppm. HRMS (ESI^+): calcd for $C_{30}H_{27}NNaO_2$ $[M+Na]^+$ 456.1939, found 456.1937.



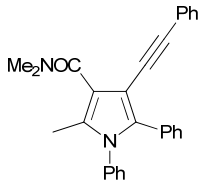
Allyl 2-methyl-1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3d)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3d** as a pale yellow solid (74.0 mg, 59% yield). M.p.: 108-110 ºC. ^1H NMR ($CDCl_3$, 400 MHz): δ = 2.42 (s, 3H), 4.88 (dt, J = 5.6 Hz, 1.2 Hz, 2H), 5.26 (dq, J = 10.4 Hz, 1.6 Hz, 1H), 5.52 (dq, J = 17.2 Hz, 1.6 Hz, 1H), 6.06-6.14 (m, 1H), 7.10-7.13 (m, 2H), 7.18-7.23 (m, 3H), 7.25-7.31 (m, 5H), 7.36-7.39 (m, 5H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.0, 64.8, 85.3, 91.6, 104.5, 113.3, 117.8, 124.6, 127.5, 127.8, 128.2, 128.6, 129.4, 130.1, 130.8, 131.3, 133.1, 137.6, 138.2, 138.3, 164.8 ppm. HRMS (ESI^+): calcd for $C_{29}H_{23}NNaO_2$ $[M+Na]^+$ 440.1626, found 440.1630.



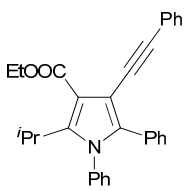
Benzyl 2-methyl-1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3e)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3e** as a pale yellow solid (103.4 mg, 74% yield). M.p.: 149-151 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.45 (s, 3H), 5.44 (s, 2H), 7.11-7.16 (m, 4H), 7.18-7.24 (m, 6H), 7.31-7.32 (m, 5H), 7.35-7.39 (m, 3H), 7.55-7.57 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.0, 65.9, 85.2, 91.6, 104.4, 113.0, 124.4, 127.37, 127.45, 127.8, 127.9, 128.1, 128.3, 128.6, 129.3, 130.1, 130.7, 131.3, 136.8, 137.6, 138.2, 138.5, 165.0 ppm. HRMS (ESI$^+$): calcd for $C_{33}H_{25}NNaO_2$ $[M+Na]^+$ 490.1783, found 490.1788.



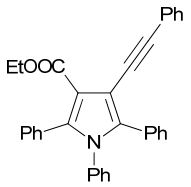
***N*,*N*,2-Trimethyl-1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxamide (3f)**

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 8/1–2/1, v/v) afforded **3f** as a pale yellow solid (42.3 mg, 35% yield). M.p.: 206-208 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.17 (s, 3H), 3.19 (s, 3H), 3.25 (s, 3H), 7.13-7.22 (m, 5H), 7.24-7.30 (m, 5H), 7.33-7.37 (m, 5H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 12.1, 35.2, 39.3, 84.9, 91.3, 103.0, 119.4, 124.4, 127.1, 127.5, 127.9, 128.2, 128.4, 128.6, 129.3, 129.7, 131.06, 131.13, 136.6, 138.2, 167.8 ppm. HRMS (ESI$^+$): calcd for $C_{28}H_{24}N_2NaO$ $[M+Na]^+$ 427.1786, found 427.1789.



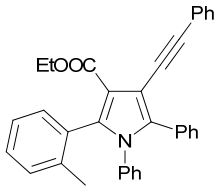
Ethyl 2-isopropyl-1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3g)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3g** as a pale yellow solid (50.7 mg, 39% yield). M.p.: 202-204 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.32 (d, J = 7.2 Hz, 6H), 1.45 (t, J = 7.2 Hz, 3H), 3.05-3.16 (m, 1H), 4.42 (q, J = 7.2 Hz, 2H), 7.12-7.18 (m, 5H), 7.23-7.28 (m, 5H), 7.35-7.36 (m, 5H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 14.7, 20.8, 27.0, 60.3, 85.1, 91.4, 105.0, 113.2, 124.7, 127.41, 127.43, 127.7, 128.3, 128.8, 129.15, 129.19, 130.4, 131.0, 131.2, 138.0, 138.1, 146.0, 165.1 ppm. HRMS (ESI$^+$): calcd for $C_{30}H_{27}NNaO_2$ $[M+Na]^+$ 456.1939, found 456.1945.



Ethyl 1,2,5-triphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3h)

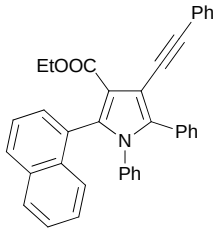
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3h** as a pale yellow solid (66.3 mg, 47% yield). M.p.: 187-189 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.20 (t, J = 7.2 Hz, 3H), 4.23 (q, J = 7.2 Hz, 2H), 6.88-6.90 (m, 2H), 7.09-7.15 (m, 3H), 7.19-7.31 (m, 11H), 7.32-7.34 (m, 2H), 7.42 (dd, J = 7.2 Hz, 1.2 Hz, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 14.3, 60.1, 84.6, 92.0, 105.2, 115.3, 124.6, 127.5, 127.6, 127.7, 127.8, 127.9, 128.1, 128.3, 128.7, 129.0, 130.4, 130.7, 131.4, 131.5, 137.6, 138.7, 139.6, 164.3 ppm. HRMS (ESI$^+$): calcd for $C_{33}H_{26}NO_2$ $[M+H]^+$ 468.1964, found 468.1960.



Ethyl 1,5-diphenyl-4-(phenylethynyl)-2-(*o*-tolyl)-1*H*-pyrrole-3-carboxylate (3i)

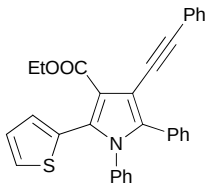
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3i** as a pale yellow solid (80.3 mg, 56% yield). M.p.: 162-164 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.12 (t, J = 7.2 Hz, 3H), 2.11 (s, 3H), 4.14-4.22 (m,

2H), 6.88 (d, J = 6.0 Hz, 2H), 7.03-7.10 (m, 6H), 7.16 (td, J = 7.2 Hz, 1.6 Hz, 1H), 7.21-7.32 (m, 6H), 7.35-7.37 (m, 2H), 7.44 (dd, J = 8.0 Hz, 1.6 Hz, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 14.2, 20.3, 59.9, 84.7, 92.1, 105.0, 115.3, 124.5, 125.0, 127.6, 127.8, 127.9, 128.3, 128.4, 128.6, 128.7, 129.4, 130.2, 130.7, 131.4, 131.5, 131.7, 137.6, 138.4, 138.5, 139.6, 164.0 ppm. HRMS (ESI$^+$): calcd for $C_{34}H_{27}NNaO_2$ $[M+Na]^+$ 504.1939, found 504.1945.



Ethyl 2-(naphthalen-1-yl)-1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3j)

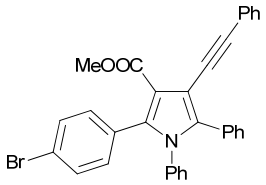
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3j** as a pale yellow solid (103.0 mg, 66% yield). M.p.: 192-194 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 0.74 (t, J = 6.8 Hz, 3H), 3.97 (q, J = 6.8 Hz, 2H), 6.85-7.03 (m, 5H), 7.21-7.33 (m, 8H), 7.40-7.49 (m, 6H), 7.75-7.80 (m, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.7, 59.7, 84.5, 92.3, 105.2, 116.7, 124.5, 124.7, 125.8, 126.0, 126.4, 127.6, 127.7, 127.86, 127.89, 128.2, 128.3, 128.5, 128.9, 129.5, 129.9, 130.3, 130.6, 131.4, 133.1, 133.8, 137.6, 137.8, 138.9, 163.8 ppm. HRMS (ESI$^+$): calcd for $C_{37}H_{27}NNaO_2$ $[M+Na]^+$ 540.1939, found 540.1935.



Ethyl 1,5-diphenyl-4-(phenylethynyl)-2-(thiophen-2-yl)-1*H*-pyrrole-3-carboxylate (3k)

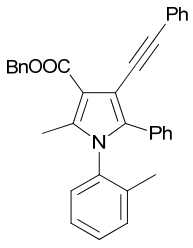
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3k** as a pale yellow solid (72.7 mg, 51% yield). M.p.: 166-168 ºC.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.27 (t, J = 7.2 Hz, 3H), 4.29 (q, J = 7.2 Hz, 2H), 6.88-6.90 (m, 1H), 6.92 (dd, J = 3.6 Hz, 1.2 Hz, 1H), 6.98-7.00 (m, 2H), 7.16-7.306 (m, 10H), 7.314-7.35 (m, 2H), 7.41 (dd, J = 7.6 Hz, 1.6 Hz, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 14.4, 60.3, 84.2, 92.1, 105.4, 117.3, 124.4, 126.3, 127.7, 127.9, 128.3, 128.8, 128.9, 130.36, 130.40, 131.0, 131.2, 131.4, 131.5, 137.5, 139.5, 164.0 ppm. HRMS (ESI$^+$): calcd for $C_{31}H_{23}NNaO_2S$ $[M+Na]^+$ 496.1347, found 496.1342.



Methyl 2-(4-bromophenyl)-1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3l)

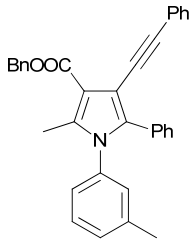
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3l** as a pale yellow solid (69.0 mg, 43% yield). M.p.: 189-191 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 3.80 (s, 3H), 6.88 (d, J = 7.2 Hz, 2H), 7.06 (d, J = 8.0 Hz, 2H), 7.13-7.20 (m, 3H), 7.23-7.25 (m, 3H), 7.28-7.32 (m, 5H), 7.35 (d, J = 8.4 Hz, 2H), 7.41-7.43 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 51.4, 84.3, 92.3, 105.3, 115.2, 122.7, 124.3, 127.7, 127.9, 128.2, 128.3, 128.8, 129.0, 130.2, 130.4, 130.8, 131.4, 133.0, 137.2, 138.2, 138.9, 164.6 ppm. HRMS (ESI$^+$): calcd for $C_{32}H_{23}BrNO_2$ $[M+H]^+$ 532.0912, found 532.0917.



Benzyl 2-methyl-5-phenyl-4-(phenylethynyl)-1-(*o*-tolyl)-1*H*-pyrrole-3-carboxylate (3m)

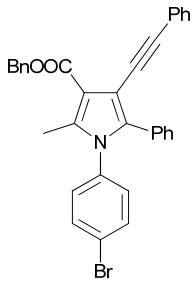
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate =

20/1, v/v) afforded **3m** as pale yellow oil (98.2 mg, 68% yield). M.p.: 153-155 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.88 (s, 3H), 2.32 (s, 3H), 5.39-5.46 (m, 2H), 7.11-7.14 (m, 2H), 7.18-7.23 (m, 8H), 7.25-7.27 (m, 1H), 7.28-7.34 (m, 6H), 7.54-7.56 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 12.6, 17.5, 66.0, 85.3, 91.6, 104.1, 112.9, 124.4, 126.9, 127.4, 127.6, 127.8, 127.9, 128.1, 128.4, 128.6, 129.3, 129.4, 129.8, 130.7, 131.2, 131.3, 136.4, 136.6, 136.8, 138.2, 138.3, 165.1 ppm. HRMS (ESI$^+$): calcd for $C_{34}H_{28}NO_2$ $[M+H]^+$ 482.2120, found 482.2114.



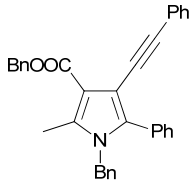
Benzyl 2-methyl-5-phenyl-4-(phenylethynyl)-1-(*m*-tolyl)-1*H*-pyrrole-3-carboxylate (3n)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3n** as a pale yellow solid (107.6 mg, 74% yield). M.p.: 131-133 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.32 (s, 3H), 2.42 (s, 3H), 5.41 (s, 2H), 6.89 (d, J = 8.0 Hz, 1H), 6.93 (s, 1H), 7.10-7.12 (m, 2H), 7.15-7.24 (m, 8H), 7.29-7.31 (m, 5H), 7.53-7.55 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.1, 21.4, 65.9, 85.3, 91.6, 104.3, 112.9, 124.5, 125.7, 127.37, 127.44, 127.8, 127.9, 128.1, 128.3, 128.6, 129.1, 129.4, 130.1, 130.8, 131.3, 136.8, 137.5, 138.3, 138.6, 139.4, 165.1 ppm. HRMS (ESI$^+$): calcd for $C_{34}H_{28}NO_2$ $[M+H]^+$ 482.2120, found 482.2120.



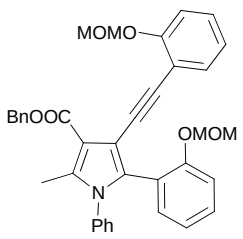
Benzyl 1-(4-bromophenyl)-2-methyl-5-phenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3o)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3o** as a pale yellow solid (117.1 mg, 71% yield). M.p.: 159-161 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.43 (s, 3H), 5.42 (s, 2H), 6.97-7.01 (m, 2H), 7.10-7.12 (m, 2H), 7.17-7.31 (m, 11H), 7.50 (d, J = 8.8 Hz, 2H), 7.53-7.54 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.0, 66.0, 84.9, 91.8, 104.8, 113.4, 122.6, 124.3, 127.5, 127.7, 127.96, 128.01, 128.1, 128.3, 128.6, 130.1, 130.2, 130.4, 131.3, 132.6, 136.6, 136.7, 138.1, 138.3, 164.9 ppm. HRMS (ESI$^+$): calcd for $C_{33}H_{24}BrNNaO_2$ $[M+Na]^+$ 568.0888, found 568.0890.



Benzyl 1-benzyl-2-methyl-5-phenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (3p)

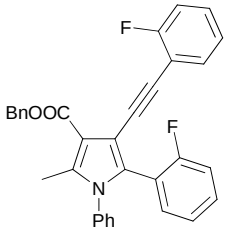
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **3p** as a pale yellow solid (72.1 mg, 50% yield). M.p.: 128-130 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.49 (s, 3H), 5.14 (s, 2H), 5.40 (s, 2H), 6.92 (d, J = 6.8 Hz, 2H), 7.05-7.06 (m, 2H), 7.15-7.19 (m, 3H), 7.24-7.33 (m, 6H), 7.35-7.39 (m, 3H), 7.43-7.45 (m, 2H), 7.52-7.55 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 12.0, 48.4, 65.9, 85.2, 91.2, 104.3, 112.8, 124.4, 125.7, 127.3, 127.6, 127.9, 128.1, 128.36, 128.39, 128.44, 128.6, 129.1, 130.4, 130.8, 131.3, 136.8, 137.1, 137.7, 139.0, 165.0 ppm. HRMS (ESI$^+$): calcd for $C_{34}H_{27}NNaO_2$ $[M+Na]^+$ 504.1939, found 504.1935.



Benzyl 5-(2-(methoxymethoxy)phenyl)-4-((2-(methoxymethoxy)phenyl)ethynyl)-

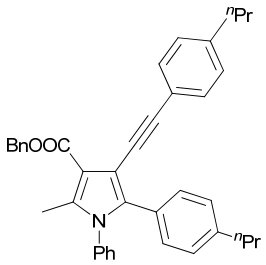
2-methyl-1-phenyl-1*H*-pyrrole-3-carboxylate (4a)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 8/1, v/v) afforded **4a** as a pale yellow solid (86.3 mg, 49% yield). M.p.: 119-121 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.45 (s, 3H), 3.26 (s, 3H), 3.28 (s, 3H), 4.77 (d, J = 6.8 Hz, 1H), 4.86 (d, J = 1.6 Hz, 2H), 4.89 (d, J = 6.8 Hz, 1H), 5.41 (s, 2H), 6.80 (td, J = 7.6 Hz, 1.2 Hz, 1H), 6.92-6.97 (m, 3H), 6.99-7.04 (m, 2H), 7.10-7.15 (m, 1H), 7.18-7.22 (m, 2H), 7.35 (dd, J = 7.6 Hz, 2.0 Hz, 1H), 7.52-7.54 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.2, 56.0, 56.1, 65.8, 87.8, 88.7, 95.1, 95.4, 105.5, 112.7, 115.1, 115.5, 116.0, 121.4, 121.5, 122.0, 127.8, 128.16, 128.19, 128.5, 128.7, 130.0, 133.3, 133.4, 135.5, 137.0, 137.6, 137.7, 156.0, 157.4, 165.1 ppm. HRMS (ESI$^+$): calcd for $C_{37}H_{33}NNaO_6$ $[M+Na]^+$ 610.2206, found 610.2207.



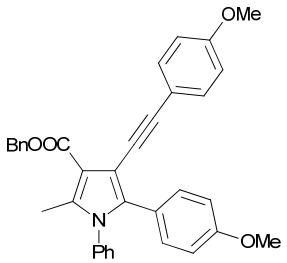
Benzyl 5-(2-fluorophenyl)-4-((2-fluorophenyl)ethynyl)-2-methyl-1-phenyl-1*H*-pyrrole-3-carboxylate (4b)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **4b** as a pale yellow solid (110.1mg, 73% yield). M.p.: 128-130 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.44 (s, 3H), 5.42 (s, 2H), 6.89 (t, J = 9.2 Hz, 1H), 6.92-7.01 (m, 3H), 7.08 (t, J = 7.6 Hz, 2H), 7.15-7.24 (m, 3H), 7.27-7.32 (m, 6H), 7.44 (t, J = 7.6 Hz, 1H), 7.52-7.54 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): 13.0, 65.9, 85.4, 89.3 (d, J = 3.0 Hz), 105.8, 112.9 (d, J = 16.0 Hz), 113.0, 115.3 (d, J = 20.0 Hz), 115.5 (d, J = 22.0 Hz), 118.9 (d, J = 15.0 Hz), 123.7 (d, J = 4.0 Hz), 123.8 (d, J = 4.0 Hz), 127.8, 128.2, 128.3, 128.5, 128.6, 129.0, 129.1, 130.4, 130.5, 133.12 (d, J = 3.0 Hz), 133.3 (d, J = 1.0 Hz), 136.8, 137.1, 138.8, 160.0 (d, J = 247.0 Hz), 162.5 (d, J = 250.0 Hz), 164.8 ppm. ^{19}F NMR ($CDCl_3$, 376 MHz): δ = -110.6, -109.9 ppm. HRMS (ESI$^+$): calcd for $C_{33}H_{23}F_2NNaO_2$ $[M+Na]^+$ 526.1595, found 526.1594.



Benzyl 2-methyl-1-phenyl-5-(4-propylphenyl)-4-((4-propylphenyl)ethynyl)-1*H*-pyrrole-3-carboxylate (4c)

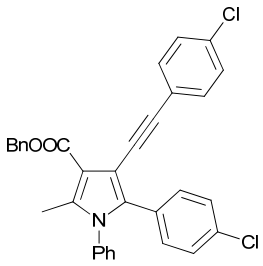
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **4c** as a pale yellow solid (102.1 mg, 62% yield). M.p.: 121-123 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 0.90 (t, J = 7.6 Hz, 3H), 0.93 (t, J = 7.6 Hz, 3H), 1.57-1.65 (m, 4H), 2.42 (s, 3H), 2.51 (t, J = 8.0 Hz, 2H), 2.55 (t, J = 8.0 Hz, 2H), 5.42 (s, 2H), 6.99-7.02 (m, 4H), 7.06 (d, J = 8.4 Hz, 2H), 7.10-7.12 (m, 2H), 7.20 (d, J = 8.0 Hz, 2H), 7.29-7.32 (m, 3H), 7.34-7.38 (m, 3H), 7.54-7.56 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.1, 13.91, 13.93, 24.4, 24.6, 37.9, 38.1, 65.9, 84.7, 91.8, 104.3, 112.9, 121.8, 127.8, 128.1, 128.27, 128.29, 128.5, 128.6, 128.7, 129.3, 129.9, 131.2, 136.9, 137.8, 138.2, 141.9, 142.1, 165.1 ppm. HRMS (ESI$^+$): calcd for $C_{39}H_{37}NNaO_2$ $[M+Na]^+$ 574.2722, found 574.2725.



Benzyl 5-(4-methoxyphenyl)-4-((4-methoxyphenyl)ethynyl)-2-methyl-1-phenyl-1*H*-pyrrole-3-carboxylate (4d)

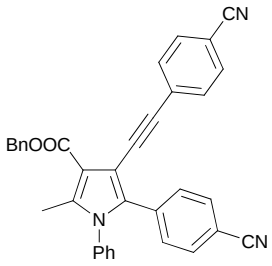
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 10/1, v/v) afforded **4d** as a pale yellow solid (84.0 mg, 53% yield). M.p.: 141-143 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.40 (s, 3H), 3.75 (s, 3H), 3.79 (s, 3H), 5.40 (s, 2H), 6.73 (dd, J = 8.8 Hz, 2.0 Hz, 4H), 7.06 (d, J = 8.8 Hz, 2H), 7.09-7.11 (m, 2H), 7.20 (d, J = 8.8 Hz, 2H), 7.28-7.31 (m, 3H), 7.36-7.38 (m, 3H), 7.53-7.54 (m, 2H) ppm. ^{13}C

NMR ($CDCl_3$, 100 MHz): δ = 13.1, 55.3, 55.4, 65.9, 83.8, 91.4, 104.1, 112.8, 113.3, 113.8, 116.8, 123.3, 127.9, 128.3, 128.55, 128.63, 128.7, 129.4, 131.4, 132.7, 136.9, 137.75, 137.82, 138.1, 158.8, 159.0, 165.2 ppm. HRMS (ESI^+): calcd for $C_{35}H_{29}NNaO_4$ $[M+Na]^+$ 550.1994, found 550.1994.



Benzyl 5-(4-chlorophenyl)-4-((4-chlorophenyl)ethynyl)-2-methyl-1-phenyl-1*H*-pyrrole-3-carboxylate (4e)

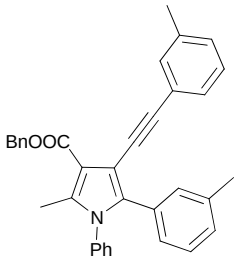
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **4e** as a pale yellow solid (91.4 mg, 57% yield). M.p.: 190-192 ºC. ^1H NMR ($CDCl_3$, 400 MHz): δ = 2.42 (s, 3H), 5.40 (s, 2H), 6.96 (dt, J = 8.8 Hz, 2.0 Hz, 2H), 7.08-7.11 (m, 2H), 7.14-7.21 (m, 6H), 7.31-7.32 (m, 3H), 7.38-7.40 (m, 3H), 7.50-7.52 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.0, 66.1, 85.8, 90.9, 104.5, 113.2, 122.7, 128.1, 128.2, 128.4, 128.5, 128.6, 128.7, 128.9, 129.2, 129.6, 131.3, 132.5, 133.4, 133.5, 136.6, 137.0, 137.3, 138.9, 164.8 ppm. HRMS (ESI^+): calcd for $C_{33}H_{23}Cl_2NNaO_2$ $[M+Na]^+$ 558.1004, found 558.1001.



Benzyl 5-(4-cyanophenyl)-4-((4-cyanophenyl)ethynyl)-2-methyl-1-phenyl-1*H*-pyrrole-3-carboxylate (4f)

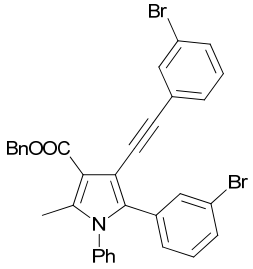
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **4f** as a pale yellow solid (63.1 mg, 41% yield). M.p.: 204-206 ºC.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.44 (s, 3H), 5.39 (s, 2H), 7.01 (d, J = 8.4 Hz, 2H), 7.10-7.12 (m, 2H), 7.32-7.37 (m, 5H), 7.42-7.44 (m, 9H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.0, 66.3, 89.1, 91.1, 105.3, 110.8, 111.1, 113.9, 118.7, 118.8, 128.2, 128.4, 128.6, 128.7, 128.8, 129.4, 129.8, 130.3, 131.6, 131.7, 131.9, 135.0, 136.4, 136.5, 136.8, 140.2, 164.4 ppm. HRMS (ESI^+): calcd for $C_{35}H_{23}N_3NaO_2$ $[M+Na]^+$ 540.1688, found 540.1690.



Benzyl 2-methyl-1-phenyl-5-(*m*-tolyl)-4-(*m*-tolylethynyl)-1*H*-pyrrole-3-carboxylate (4g)

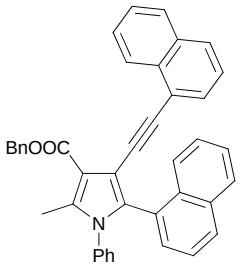
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **4g** as a pale yellow solid (108.8 mg, 73% yield). M.p.: 117-119 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.23 (s, 3H), 2.25 (s, 3H), 2.42 (s, 3H), 5.42 (s, 2H), 6.93-7.13 (m, 9H), 7.21 (s, 1H), 7.29-7.31 (m, 3H), 7.36-7.39 (m, 3H), 7.54 (dd, J = 7.2 Hz, 1.6 Hz, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.1, 21.4, 21.5, 65.9, 85.0, 92.0, 104.4, 113.0, 124.4, 127.1, 127.6, 127.9, 128.0, 128.2, 128.3, 128.5, 128.57, 128.60, 128.7, 129.3, 130.6, 131.0, 131.9, 136.9, 137.2, 137.67, 137.73, 138.4, 165.1 ppm. HRMS (ESI^+): calcd for $C_{35}H_{29}NNaO_2$ $[M+Na]^+$ 518.2096, found 518.2098.



Benzyl 5-(3-bromophenyl)-4-((3-bromophenyl)ethynyl)-2-methyl-1-phenyl-1*H*-

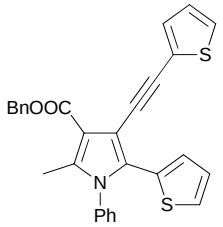
pyrrole-3-carboxylate (4h)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **4h** as a pale yellow solid (104.0 mg, 55% yield). M.p.: 122-124 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.43 (s, 3H), 5.41 (s, 2H), 6.99-7.08 (m, 4H), 7.11-7.13 (m, 2H), 7.31-7.36 (m, 6H), 7.39-7.43 (m, 3H), 7.51-7.54 (m, 2H), 7.64-7.65 (m, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.0, 66.1, 86.2, 90.9, 104.8, 113.3, 121.9, 122.0, 126.1, 128.19, 128.24, 128.3, 128.5, 128.7, 129.0, 129.3, 129.6, 130.0, 130.6, 130.7, 132.5, 133.0, 133.9, 136.5, 136.7, 137.2, 139.1, 164.7 ppm. HRMS (ESI$^+$): calcd for $C_{33}H_{23}Br_2NNaO_2$ $[M+Na]^+$ 647.9973, found 647.9980.



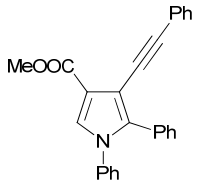
Benzyl 2-methyl-5-(naphthalen-1-yl)-4-(naphthalen-1-ylethynyl)-1-phenyl-1*H*-pyrrole-3-carboxylate (4i)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **4i** as a pale yellow solid (89.3 mg, 52% yield). M.p.: 137-139 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.54 (s, 3H), 5.46 (d, J = 12.4 Hz, 1H), 5.56 (d, J = 12.4 Hz, 1H), 6.87-6.98 (m, 4H), 7.14 (t, J = 8.0 Hz, 2H), 7.19 (t, J = 6.8 Hz, 2H), 7.28-7.37 (m, 7H), 7.45-7.48 (m, 2H), 7.57-7.60 (m, 3H), 7.64 (d, J = 8.4 Hz, 1H), 7.83 (d, J = 7.6 Hz, 1H), 7.86-7.89 (m, 1H), 8.00-8.02 (m, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 13.2, 66.0, 89.4, 90.7, 106.8, 112.6, 121.8, 125.1, 125.9, 126.06, 126.13, 126.3, 126.5, 126.7, 127.5, 127.8, 127.9, 128.2, 128.4, 128.5, 128.7, 128.98, 129.01, 129.1, 129.5, 130.1, 132.9, 133.0, 133.1, 133.6, 136.87, 136.93, 137.2, 138.3, 165.1 ppm. HRMS (ESI$^+$): calcd for $C_{41}H_{29}NNaO_2$ $[M+Na]^+$ 590.2096, found 590.2095.



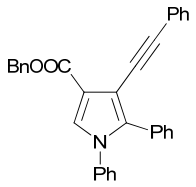
Benzyl 2-methyl-1-phenyl-5-(thiophen-2-yl)-4-(thiophen-2-ylethynyl)-1*H*-pyrrole-3-carboxylate (4j)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **4j** as a pale yellow solid (55.7 mg, 39% yield). M.p.: 148-149 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.36 (s, 3H), 5.41 (s, 2H), 6.86 (t, J = 4.4 Hz, 1H), 6.94-6.97 (m, 2H), 7.00-7.01 (m, 1H), 7.15 (d, J = 5.2 Hz, 1H), 7.20-7.23 (m, 3H), 7.27-7.32 (m, 3H), 7.44-7.48 (m, 3H), 7.53 (d, J = 7.2 Hz, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 12.9, 65.9, 87.1, 89.1, 104.2, 113.1, 124.6, 125.9, 126.5, 126.7, 127.0, 127.6, 127.9, 128.2, 128.6, 129.1, 129.5, 129.7, 131.1, 132.0, 132.1, 136.7, 137.3, 139.0, 164.6 ppm. HRMS (ESI$^+$): calcd for $C_{29}H_{22}NO_2S_2$ $[M+H]^+$ 480.1092, found 480.1095.



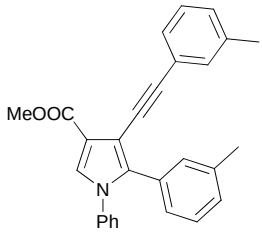
Methyl 1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (5a)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **5a** as a pale yellow solid (42.8 mg, 57% yield). M.p.: 184-186 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 3.92 (s, 3H), 7.13-7.16 (m, 2H), 7.26-7.31 (m, 6H), 7.32-7.36 (m, 5H), 7.45 (dd, J = 7.2 Hz, 1.2 Hz, 2H), 7.55 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 51.5, 84.0, 92.4, 105.8, 117.3, 124.3, 125.8, 127.7, 127.9, 128.0, 128.1, 128.3, 128.8, 129.4, 130.1, 130.3, 131.5, 138.2, 139.2, 164.4 ppm. HRMS (ESI$^+$): calcd for $C_{26}H_{19}NNaO_2$ $[M+Na]^+$ 400.1313, found 400.1317.



Benzyl 1,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrole-3-carboxylate (5b)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **5b** as a pale yellow solid (41.2 mg, 45% yield). M.p.: 136-138 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 5.40 (s, 2H), 7.13-7.15 (m, 2H), 7.24-7.30 (m, 8H), 7.32-7.35 (m, 8H), 7.49-7.51 (m, 2H), 7.60 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 66.1, 84.1, 92.4, 105.8, 117.2, 124.2, 125.8, 127.7, 127.9, 127.98, 128.05, 128.1, 128.2, 128.3, 128.7, 129.1, 129.4, 130.1, 130.3, 131.5, 136.6, 138.4, 139.2, 163.9 ppm. HRMS (ESI$^+$): calcd for $C_{32}H_{23}NNaO_2$ $[M+Na]^+$ 476.1626, found 476.1632.

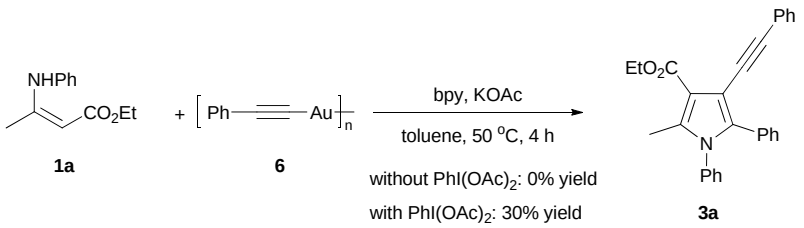


Methyl 1-phenyl-5-(*m*-tolyl)-4-(*m*-tolylethynyl)-1*H*-pyrrole-3-carboxylate (5c)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1, v/v) afforded **5c** as a pale yellow solid (37.8 mg, 47% yield). M.p.: 116-118 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.29 (s, 3H), 2.32 (s, 3H), 3.92 (s, 3H), 7.03 (d, J = 7.6 Hz, 1H), 7.08 (d, J = 7.6 Hz, 2H), 7.12-7.16 (m, 3H), 7.19 (d, J = 7.2 Hz, 1H), 7.24 (s, 1H), 7.28 (s, 2H), 7.31-7.37 (m, 3H), 7.54 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 21.4, 21.6, 51.5, 83.8, 92.7, 105.7, 117.2, 124.1, 125.7, 127.1, 127.86, 127.90, 128.2, 128.5, 128.6, 128.7, 129.4, 130.1, 130.8, 132.0, 137.6, 137.9, 138.3, 139.3, 164.4 ppm. HRMS (ESI$^+$): calcd for $C_{28}H_{24}NO_2$ $[M+H]^+$ 406.1807, found 406.1807.

VIII. Mechanism study

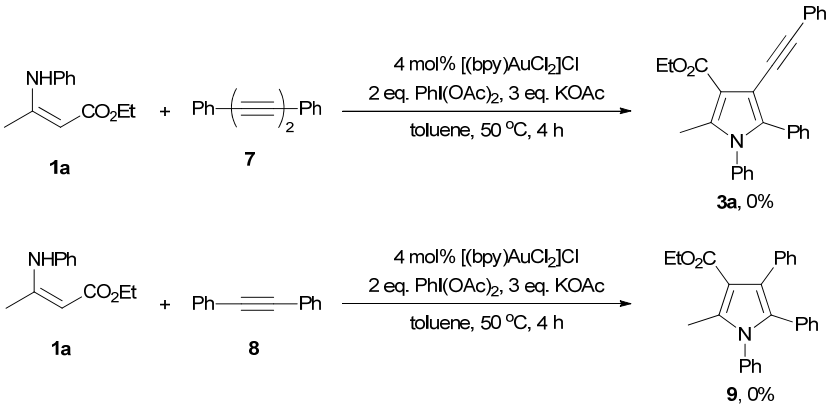
1. The reaction of enamino ester 1a with gold(I)-acetylide 6



A flame-dried sealable tube with a magnetic stir bar was charged with (*Z*)-ethyl 3-(phenylamino)but-2-enoate **1a** (97.7 μL, 0.5 mmol), gold(I)-acetylide **6**[7] (59.6 mg, 0.2 mmol), bpy (156.2 mg, 1.0 mmol), $PhI(OAc)_2$ (128.8 mg, 0.4 mmol), KOAc (58.9 mg, 0.6 mmol), and toluene (1.0 mL) under an N_2 atmosphere. The tube was sealed and the resulting mixture was stirred at 50 °C for 4 h. After being cooled to ambient temperature, the reaction solution was diluted with 20 mL of CH_2Cl_2, filtered through a celite pad and washed with 10 mL of CH_2Cl_2. The filtrate was evaporated and the residue was purified by column chromatography on silica gel (petroleum ether/ether = 20/1, v/v) to afford 12.1 mg of **3a** (30% yield).

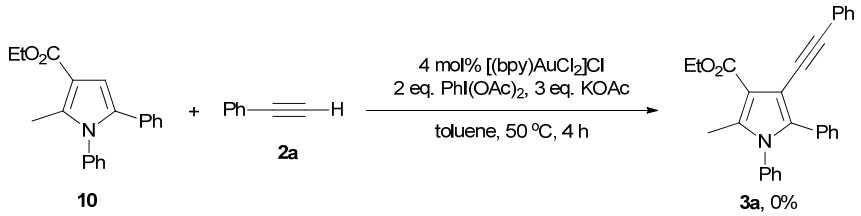
When the reaction was carried out in the absence of $PhI(OAc)_2$, no desired **3a** was observed.

2. The reaction of enamino ester 1a with internal alkynes



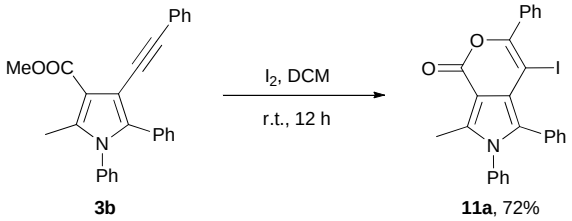
A flame-dried sealable tube with a magnetic stir bar was charged with (*Z*)-ethyl 3-(phenylamino)but-2-enoate **1a** (1.5 mmol), 1,4-diphenylbuta-1,3-diyne **7** (121.4 mg, 0.6 mmol) or 1,2-diphenylacetylene **8** (121.4 mg, 0.6 mmol)), $[(bpy)AuCl_2]Cl$ (11.1 mg, 0.024 mmol), KOAc (176.7 mg, 1.8 mmol), $PhI(OAc)_2$ (386.5 mg, 1.2 mmol), and toluene (3.0 mL) under an N_2 atmosphere. The tube was sealed and the reaction mixture was stirred at 50 °C for 4 h. No **3a** or **9** was formed.

3. The reaction of C3-unsubstituted pyrrole 10 with phenylacetylene 2a



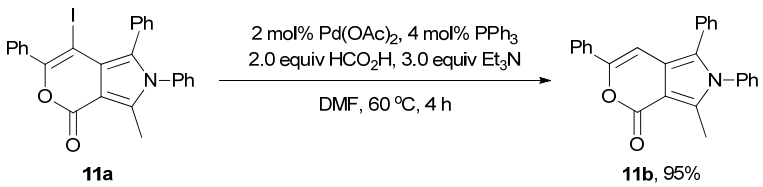
A flame-dried sealable tube with a magnetic stir bar was charged with pyrrole **10**[8] (182.3 mg, 0.6 mmol), phenylacetylene **2a** (65.9 μL, 0.6 mmol), $[(bpy)AuCl_2]Cl$ (11.1 mg, 0.024 mmol), KOAc (176.7 mg, 1.8 mmol), $PhI(OAc)_2$ (386.5 mg, 1.2 mmol), and toluene (3.0 mL) under an N_2 atmosphere. The tube was sealed and the reaction mixture was stirred at 50 °C for 4 h. No desired **3a** was formed.

IX. The derivation of 3-alkynylpyrroles



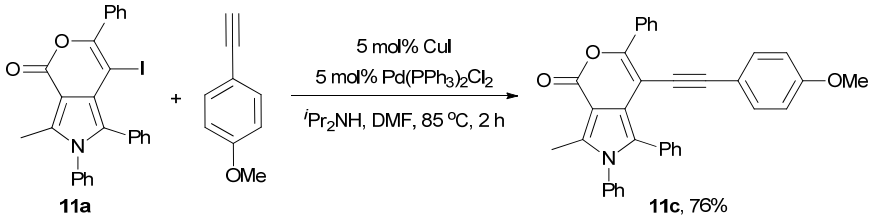
7-Iodo-3-methyl-1,2,6-triphenylpyrano[3,4-*c*]pyrrol-4(2*H*)-one (11a)[9]

A solution of I_2 (76.2 mg, 0.3 mmol) in DCM (1.5 mL) was added to a solution of **3b** (39.1 mg, 0.1 mmol) in DCM (1.5 mL) and the resulting mixture was stirred at room temperature for 12 h. The reaction mixture was diluted with DCM (10 mL), washed with $NaHSO_3$, and dried over anhydrous Na_2SO_4. The solvent was evaporated and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 8/1, v/v) to afford **11a** as a pale yellow solid (36.3 mg, 72% yield). M.p.: >250 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.54 (s, 3H), 7.06-7.07 (m, 2H), 7.17-7.25 (m, 5H), 7.31-7.32 (m, 3H), 7.39-7.42 (m, 3H), 7.61 (d, J = 7.2 Hz, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 12.2, 64.9, 105.6, 120.7, 127.3, 128.0, 128.5, 128.6, 129.0, 129.2, 129.4, 129.9, 130.3, 133.8, 135.4, 136.1, 136.7, 151.7, 160.6 ppm. HRMS (ESI$^+$): calcd for $C_{26}H_{18}INNaO_2$ $[M+Na]^+$ 526.0280, found 526.0277.



3-Methyl-1,2,6-triphenylpyrano[3,4-*c*]pyrrol-4(2*H*)-one (11b)[10]

A flame-dried sealable tube with a magnetic stir bar was charged with **11a** (50.3 mg, 0.1 mmol), $Pd(OAc)_2$ (0.5 mg, 0.002 mmol), PPh_3 (1.1 mg, 0.004 mmol), formic acid (7.5 μL, 0.2 mmol), Et_3N (41.7 μL, 0.3 mmol), and DMF (1.5 mL) under an N_2 atmosphere. The tube was sealed and the reaction mixture was stirred at 60 °C for 4 h. After being cooled to ambient temperature, the reaction solution was diluted with 10 mL of CH_2Cl_2, filtered through a celite pad, and washed with 30 mL of CH_2Cl_2. The filtrate was evaporated, and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 8/1, v/v) to afford **11b** as a pale yellow solid (36.0 mg, 95% yield). M.p.: 227-229 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.59 (s, 3H), 6.89 (s, 1H), 7.10-7.12 (m, 2H), 7.16-7.18 (m, 2H), 7.21-7.28 (m, 3H), 7.31-7.35 (m, 1H), 7.38-7.42 (m, 5H), 7.81-7.83 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 12.4, 96.5, 106.4, 120.6, 124.9, 126.9, 127.2, 128.3, 128.5, 128.6, 128.7, 128.8, 129.5, 129.6, 130.8, 133.5, 136.3, 137.3, 151.4, 160.9 ppm. HRMS (ESI^+): calcd for $C_{26}H_{19}NNaO_2$ $[M+Na]^+$ 400.1313, found 400.1315.



7-((4-Methoxyphenyl)ethynyl)-3-methyl-1,2,6-triphenylpyrano[3,4-*c*]pyrrol-4(2*H*)-one (11c)[9]

A flame-dried sealable tube with a magnetic stir bar was charged with **11a** (25.2 mg, 0.05 mmol), $(PPh_3)_2PdCl_2$ (2.0 mg, 5 mol%), CuI (0.5 mg, 5 mol%), 1-ethynyl-4-methoxybenzene (25.9 μL, 0.2 mmol), $^i Pr_2NH$ (0.5 mL), and DMF (1.0 mL) under an N_2 atmosphere. The tube was sealed and the reaction mixture was stirred at 85 °C for

2 h. After being cooled to ambient temperature, the reaction solution was diluted with 10 mL of CH_2Cl_2, filtered through a celite pad, and washed with 30 mL of CH_2Cl_2. The filtrate was collected and evaporated, and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 8/1, v/v) to provide **11c** as a pale yellow solid (19.2 mg, 76% yield). M.p.: 223-225 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.56 (s, 3H), 3.75 (s, 3H), 6.61-6.67 (m, 4H), 7.06-7.09 (m, 2H), 7.13-7.20 (m, 3H), 7.22-7.24 (m, 2H), 7.32-7.34 (m, 3H), 7.38-7.45 (m, 3H), 8.12-8.14 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 12.4, 55.3, 83.3, 96.2, 96.4, 105.2, 113.6, 115.4, 118.5, 127.4, 127.75, 127.85, 128.5, 128.6, 128.8, 128.9, 129.2, 130.7, 132.4, 132.6, 133.6, 135.8, 137.0, 154.5, 159.4, 160.0 ppm. HRMS (ESI$^+$): calcd for $C_{35}H_{26}NO_3$ $[M+H]^+$ 508.1913, found 508.1909.

X. References

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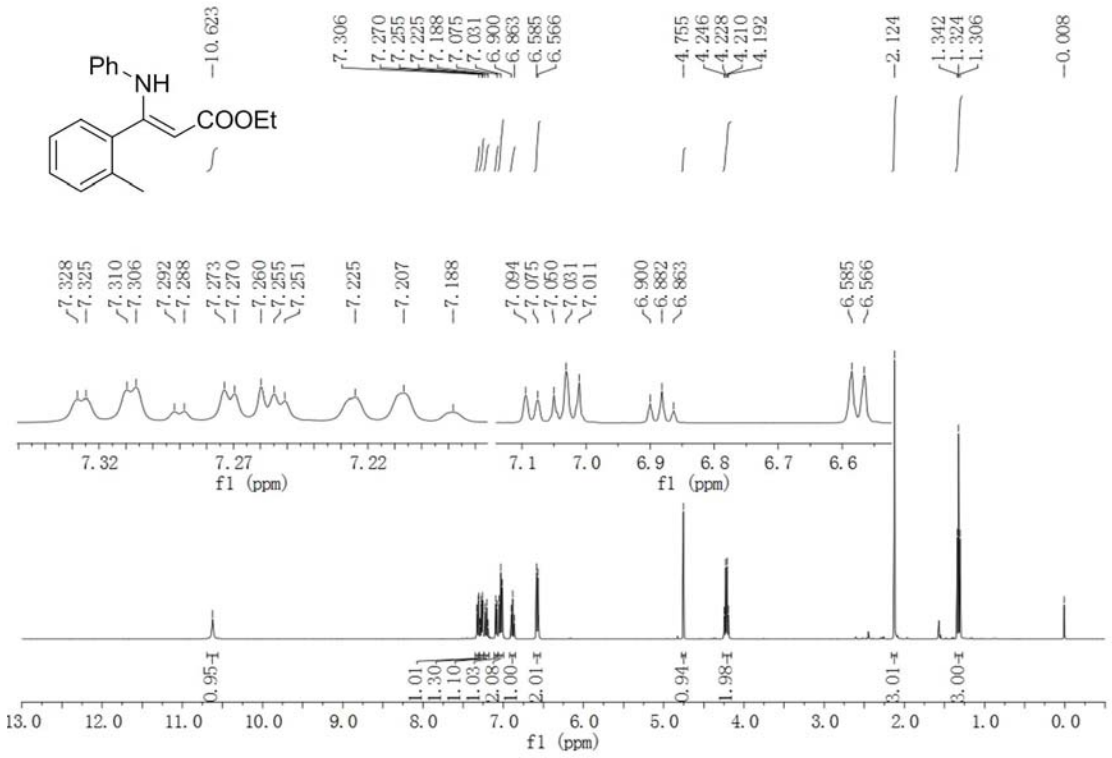
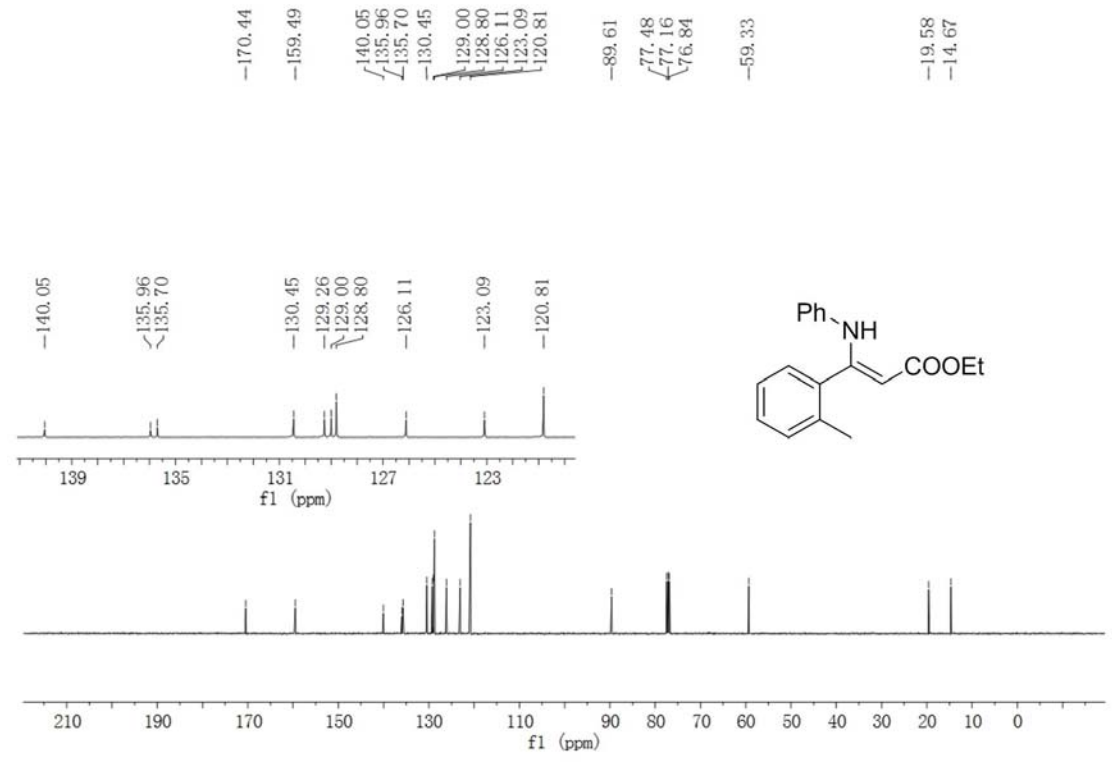
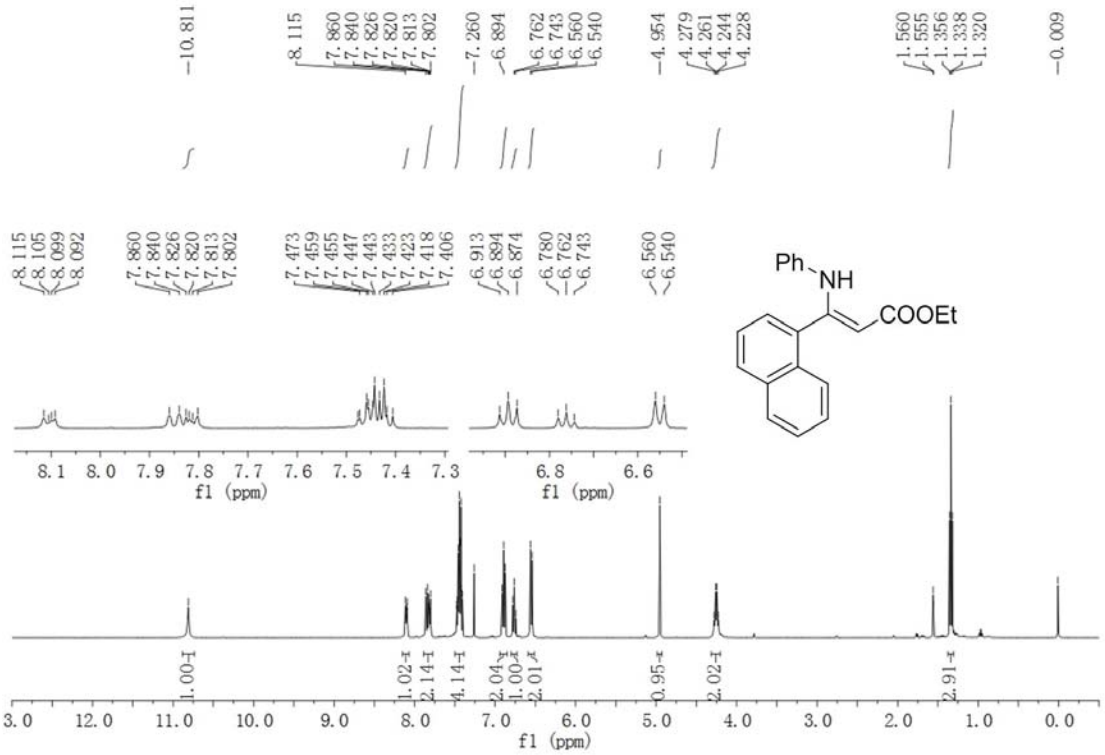
XI. Copies of ^{1}H, ^{13}C and ^{19}F NMR spectra



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6.560
6.540
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4.279
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4.244
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1.356
1.338
1.320
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4.14
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1.00
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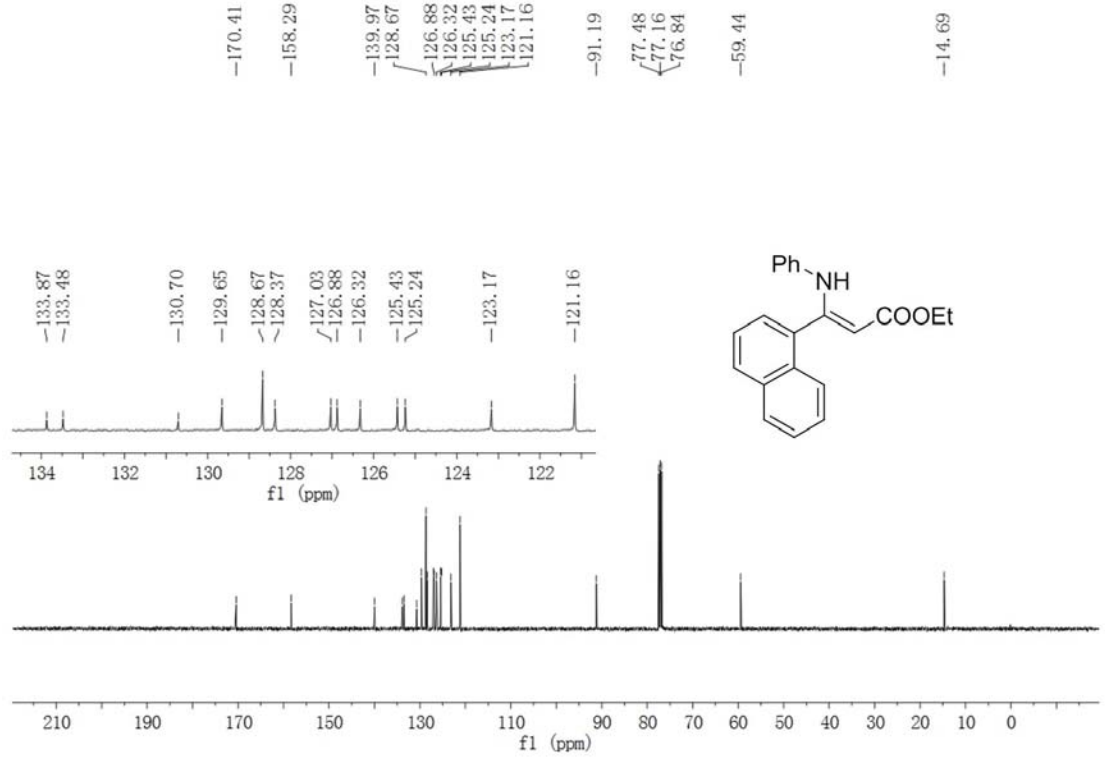
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126.32
125.43
125.24
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77.16
76.84
59.44
14.69
133.87
133.48
130.70
129.65
128.67
128.37
127.03
126.88
126.32
125.43
125.24
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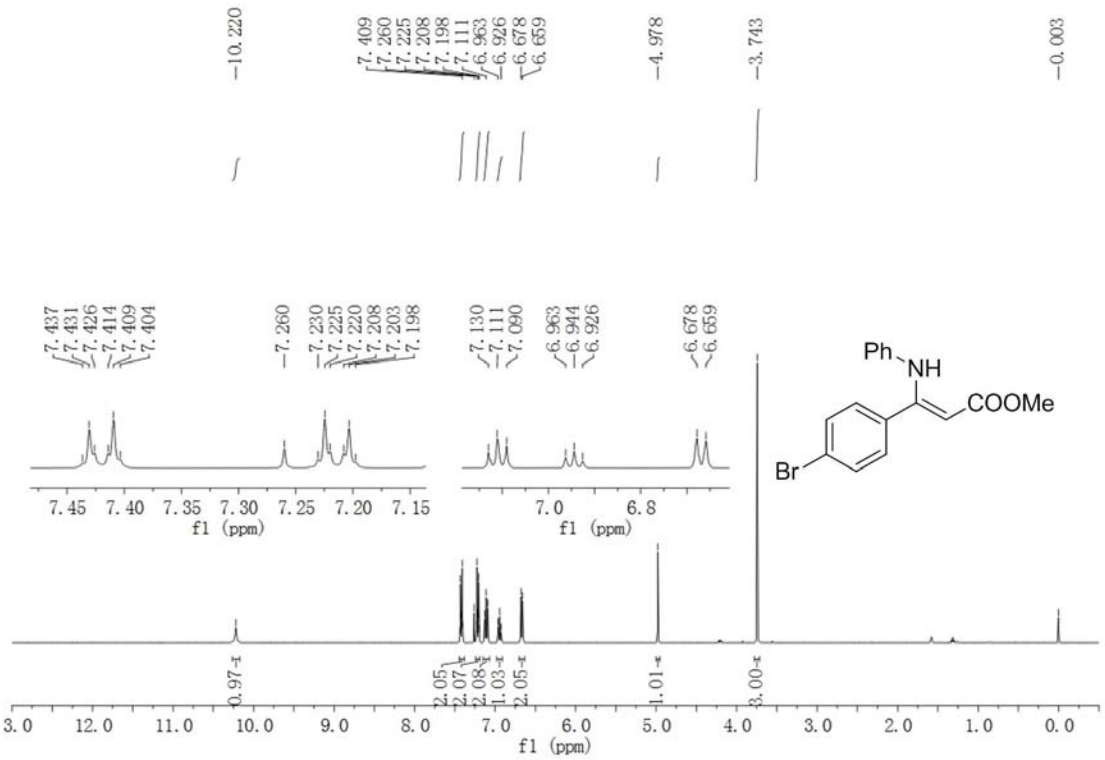
121.16
Ph
NH
COOEt
f1 (ppm)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7.198
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6.659
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3.743
0.003
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7.431
7.426
7.414
7.409
7.404
7.260
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7.225
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7.198
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6.659
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Br
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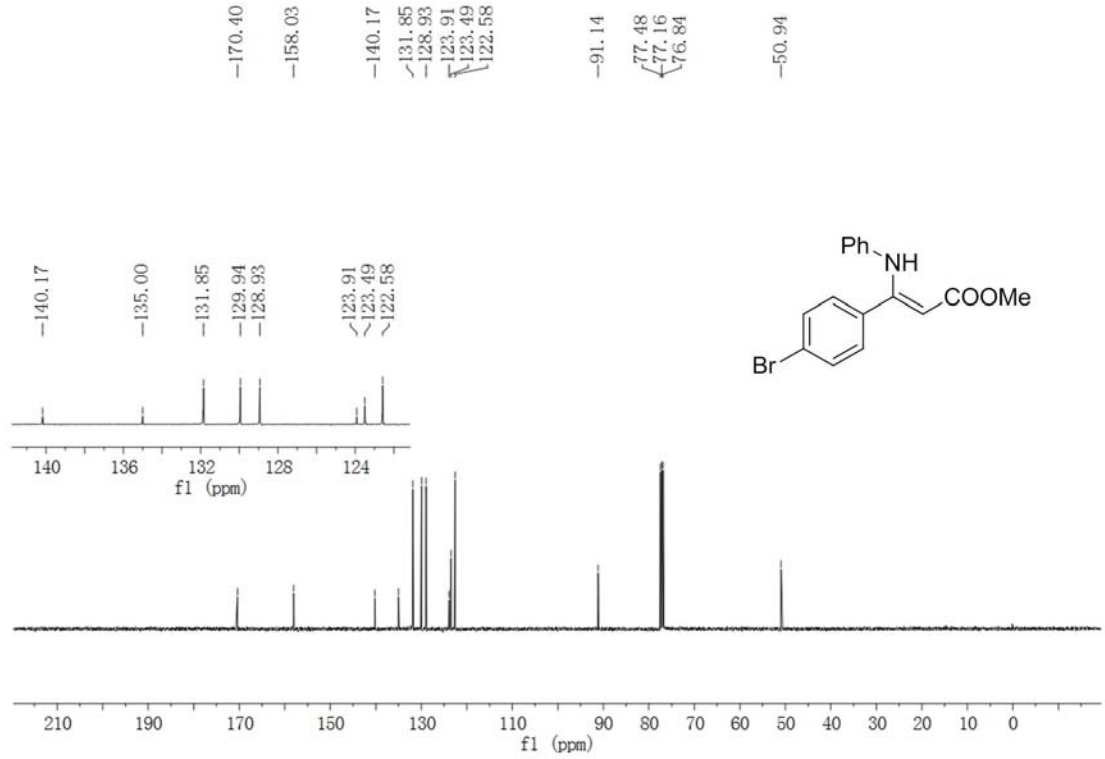
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COOMe
Br
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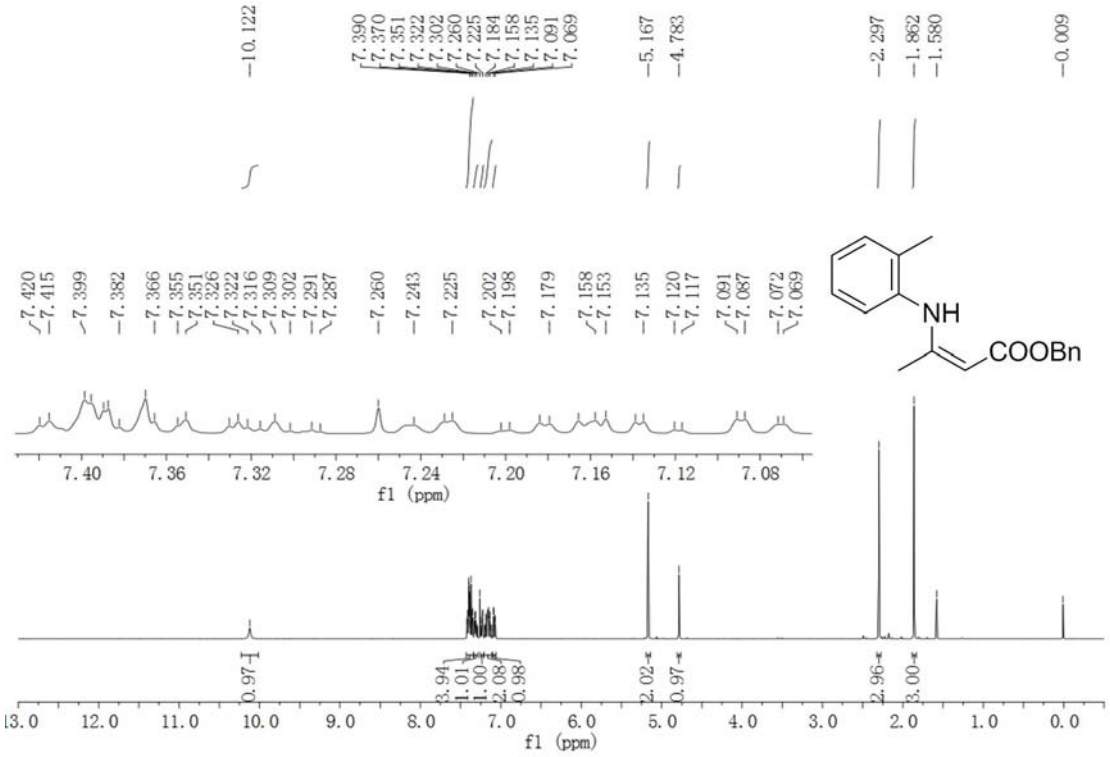
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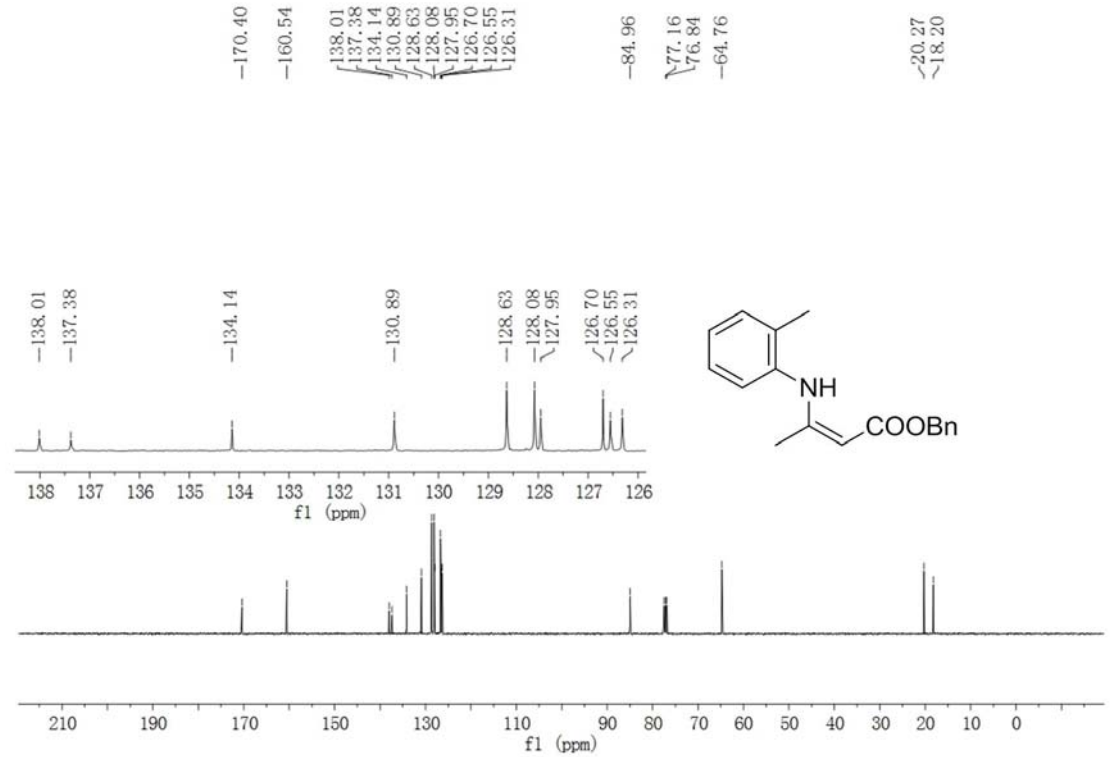
f1 (ppm)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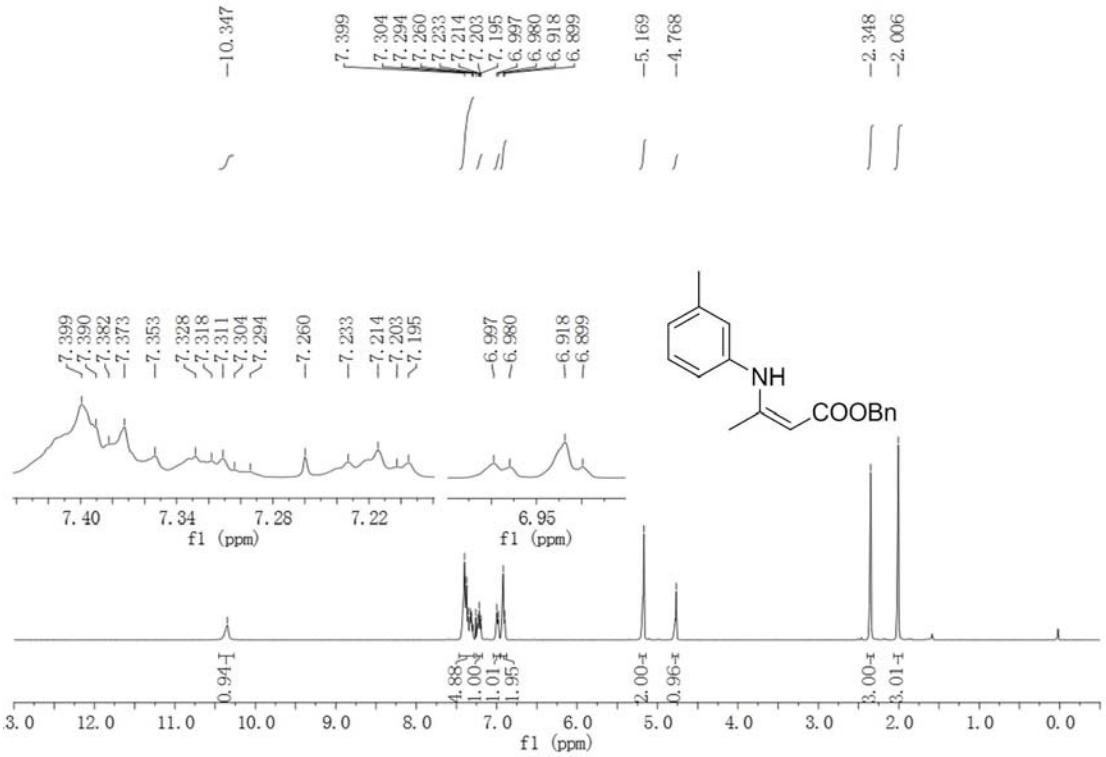
f1 (ppm)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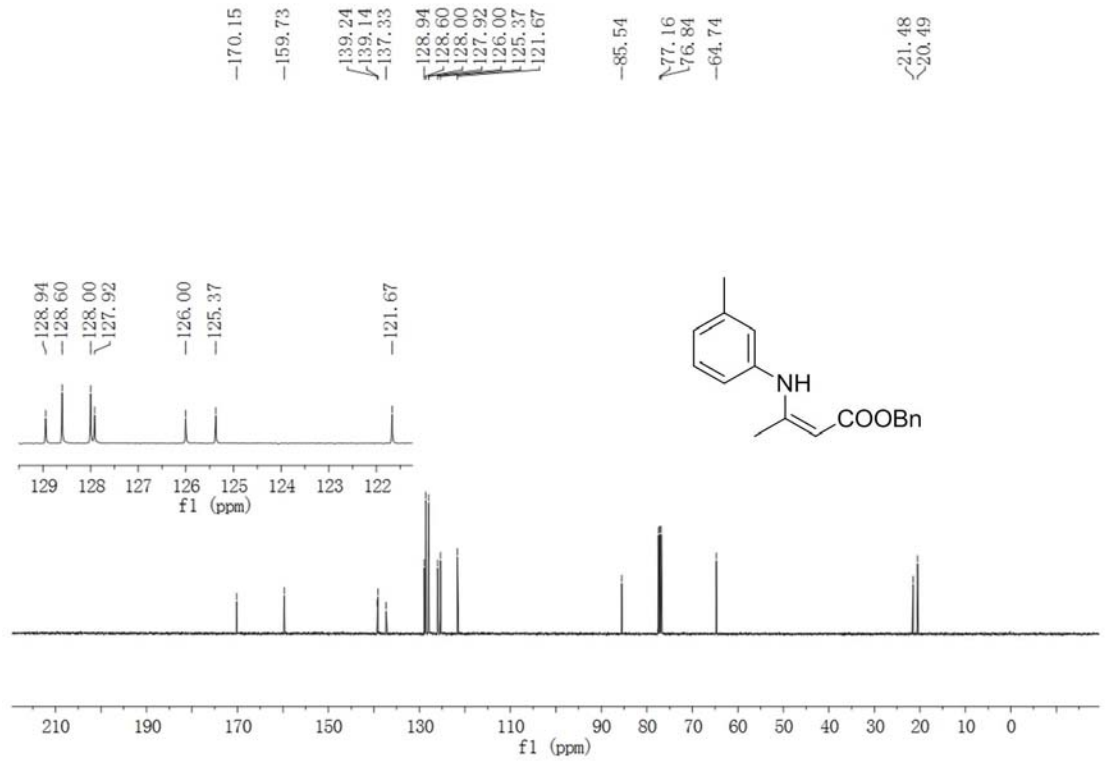
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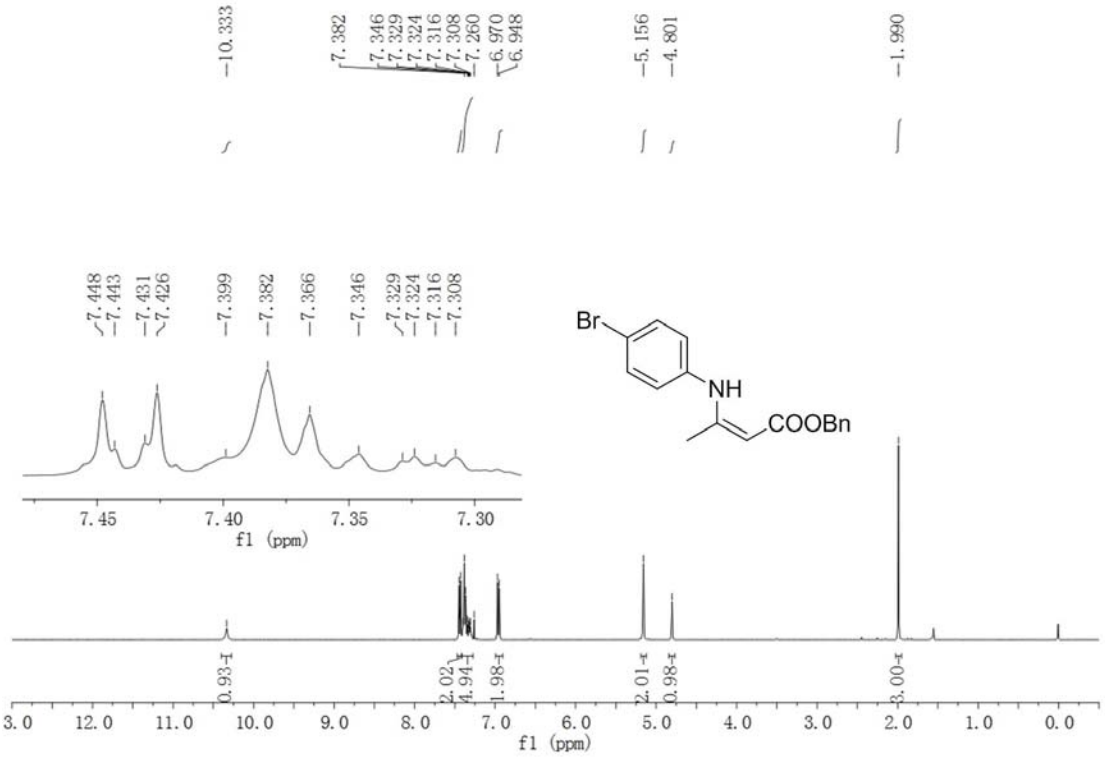
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7.431
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7.399
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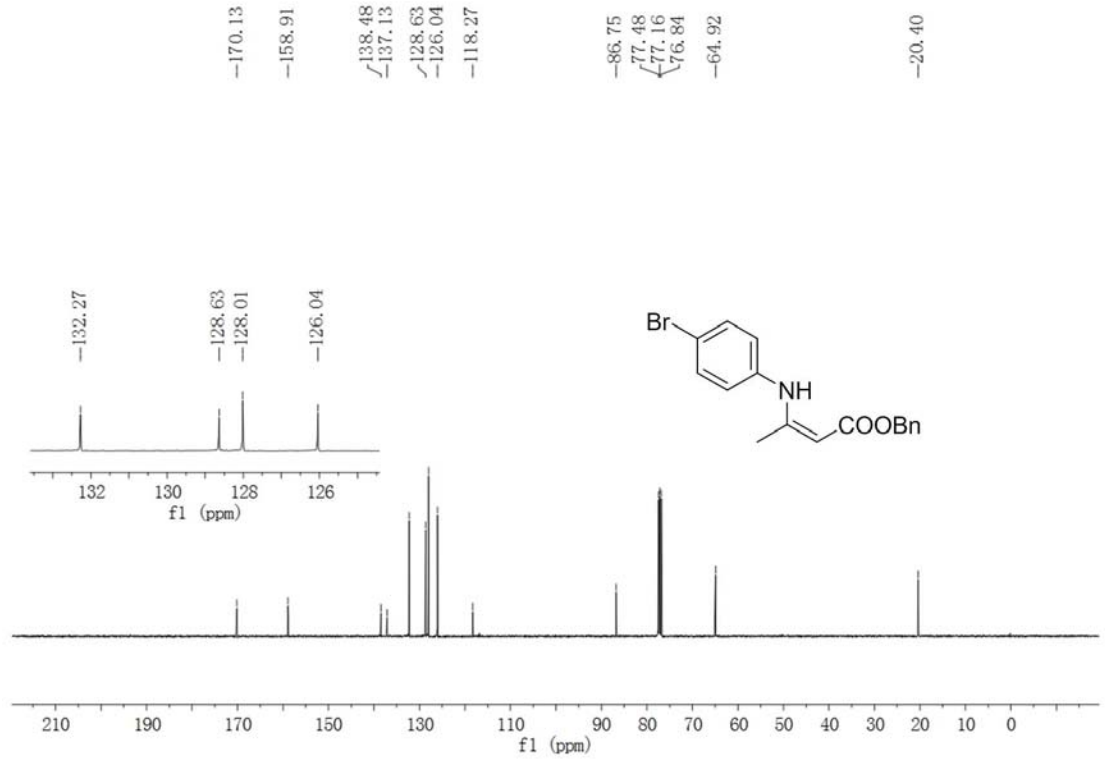
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NH
COOBn
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130
128
126
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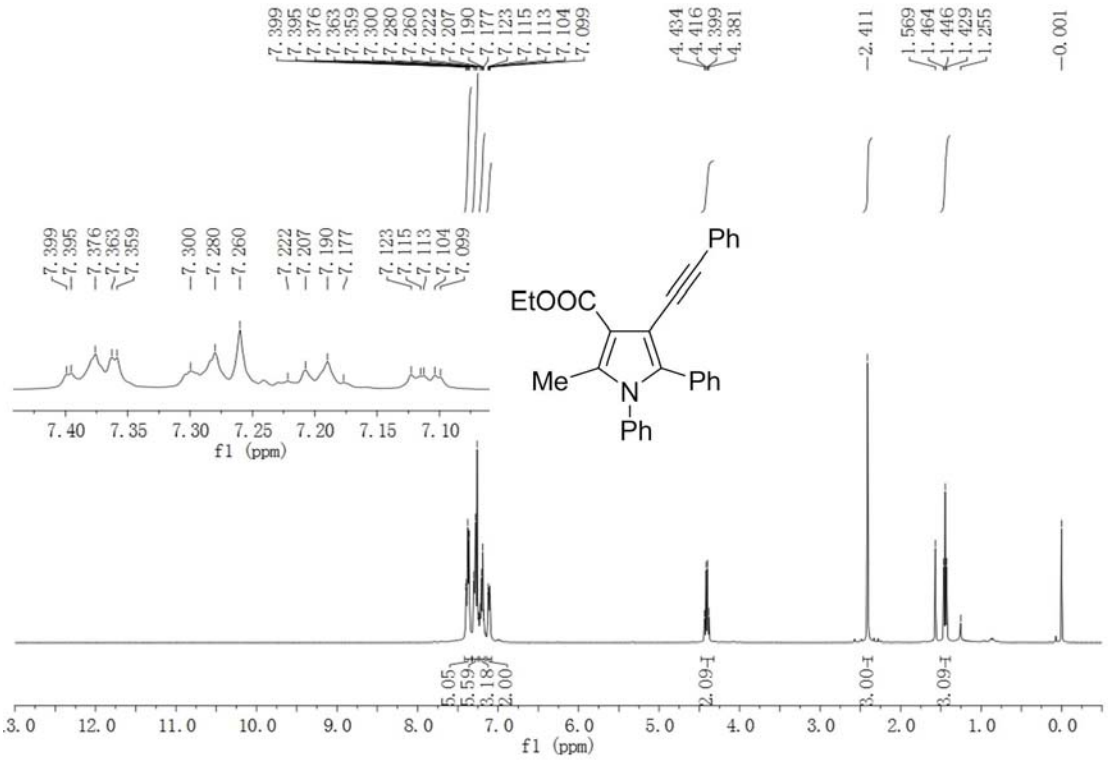
f1 (ppm)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N
Ph
Ph
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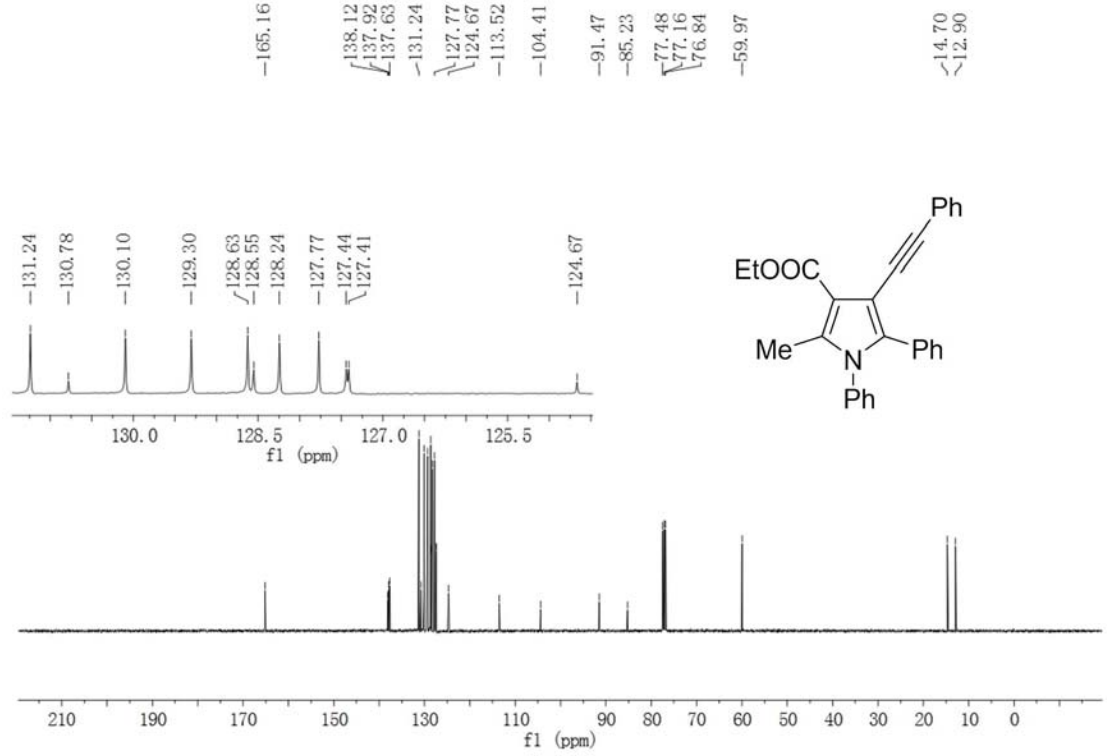
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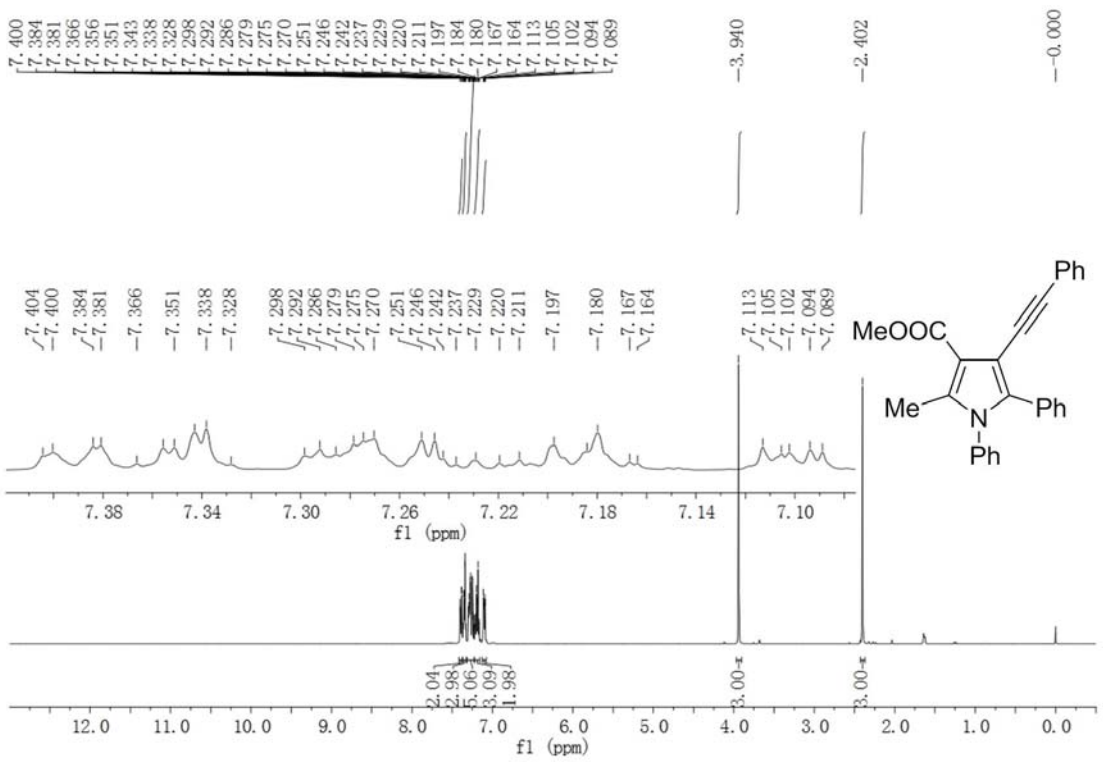
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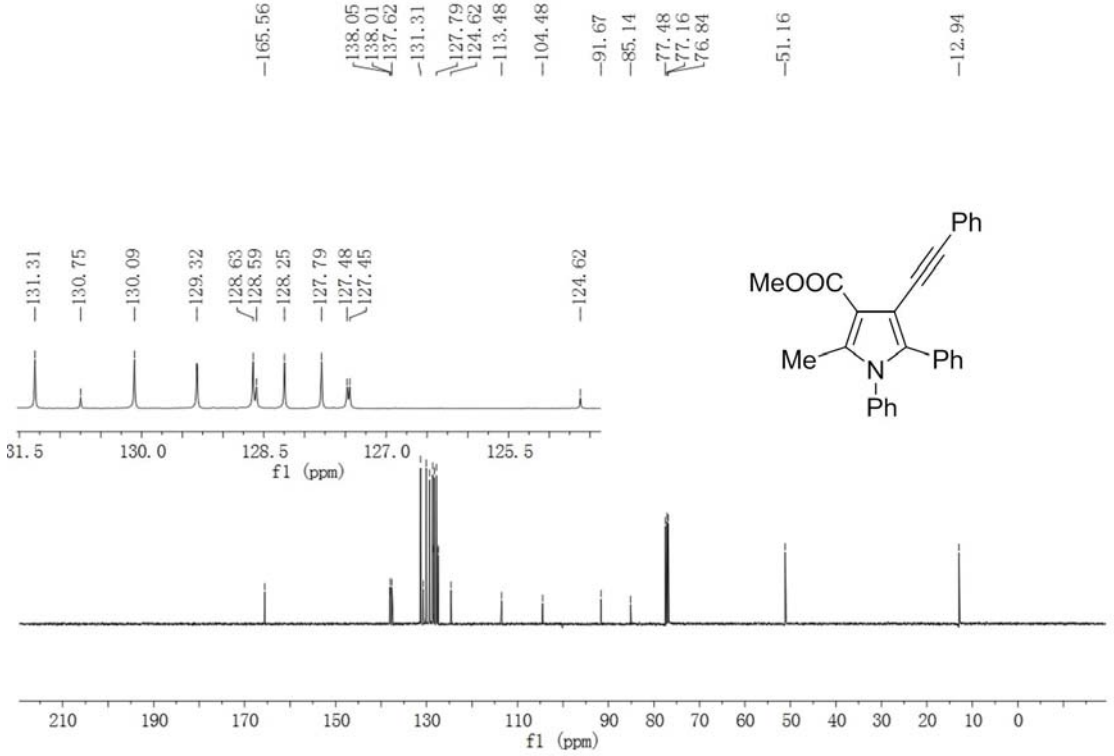
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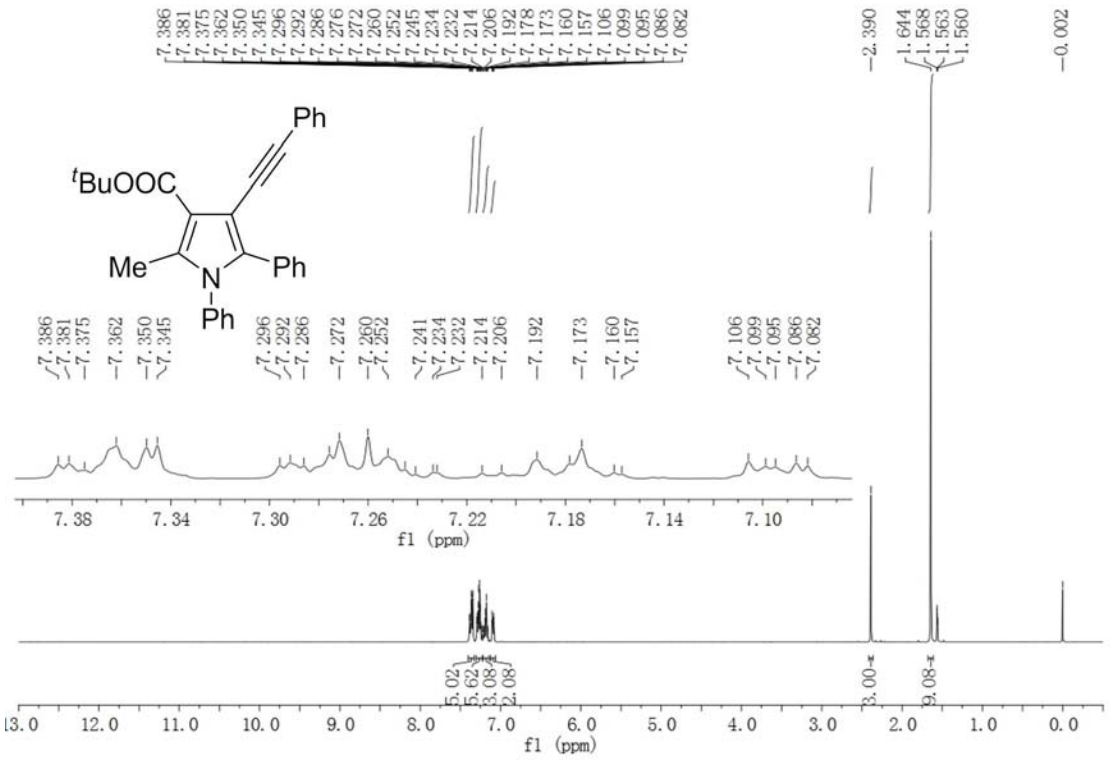
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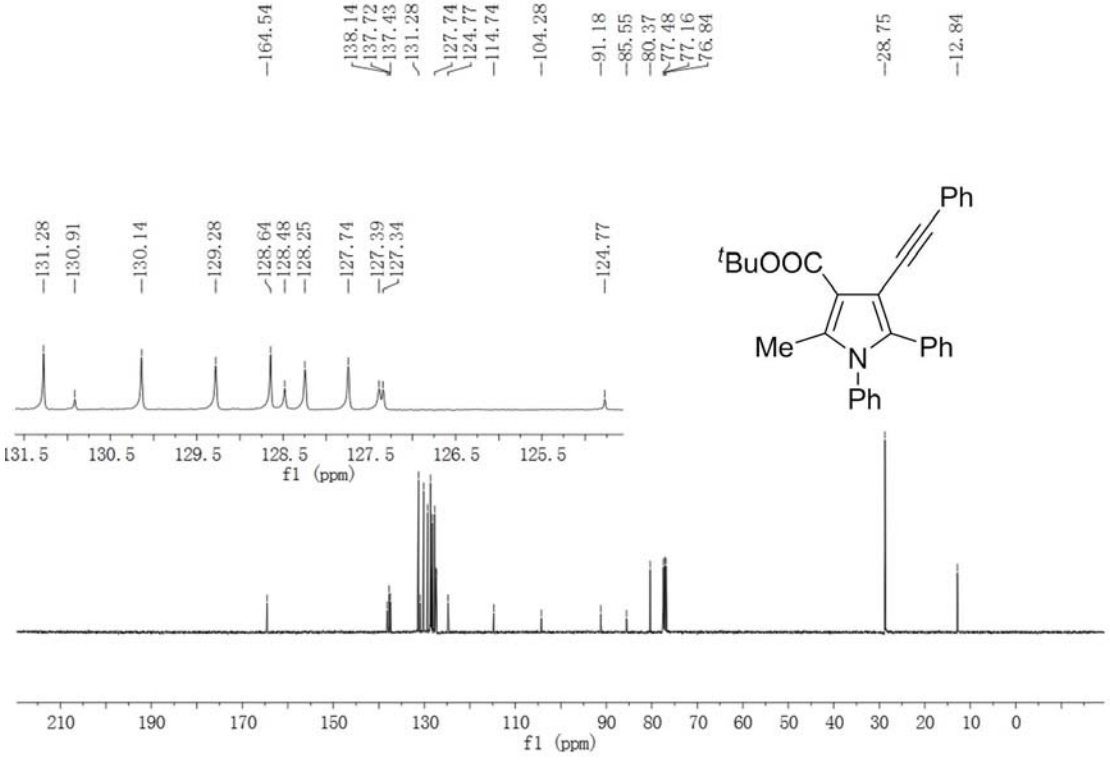
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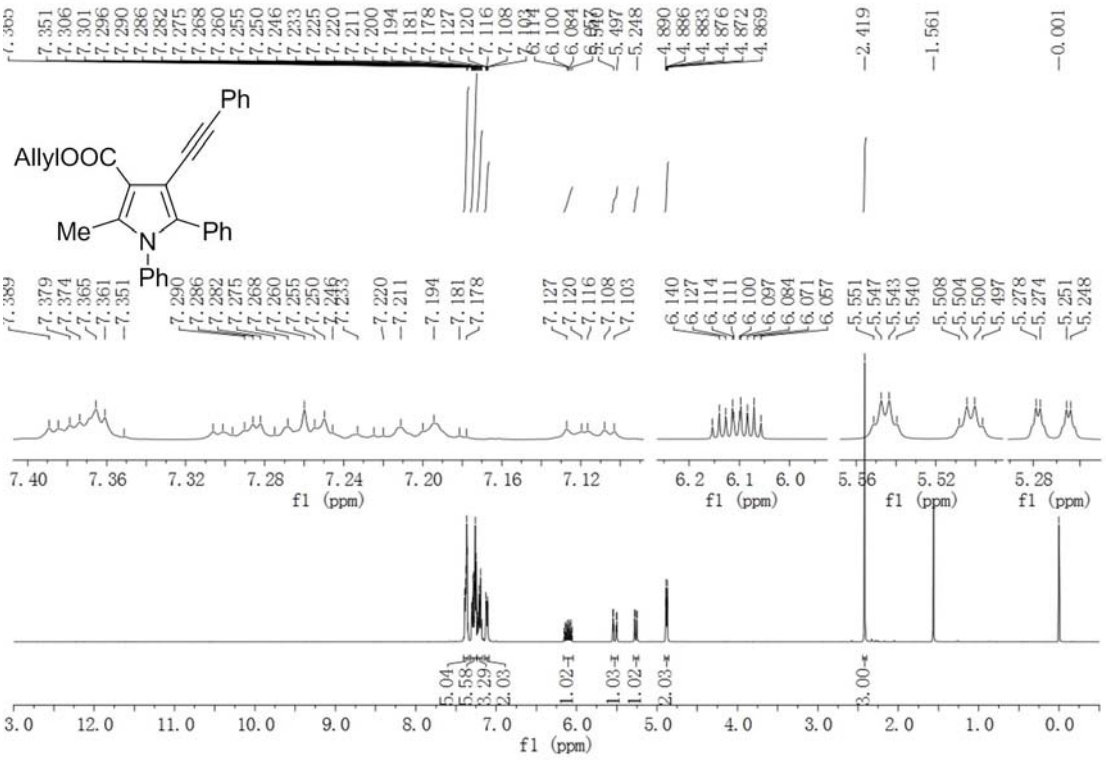
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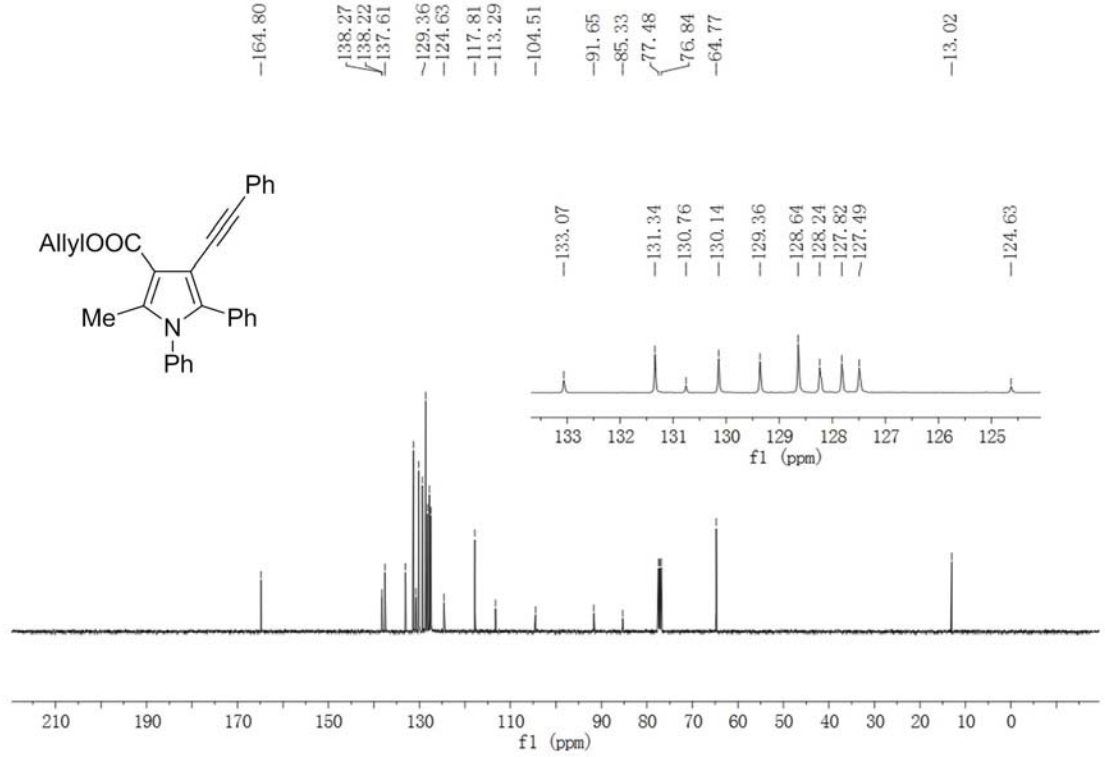
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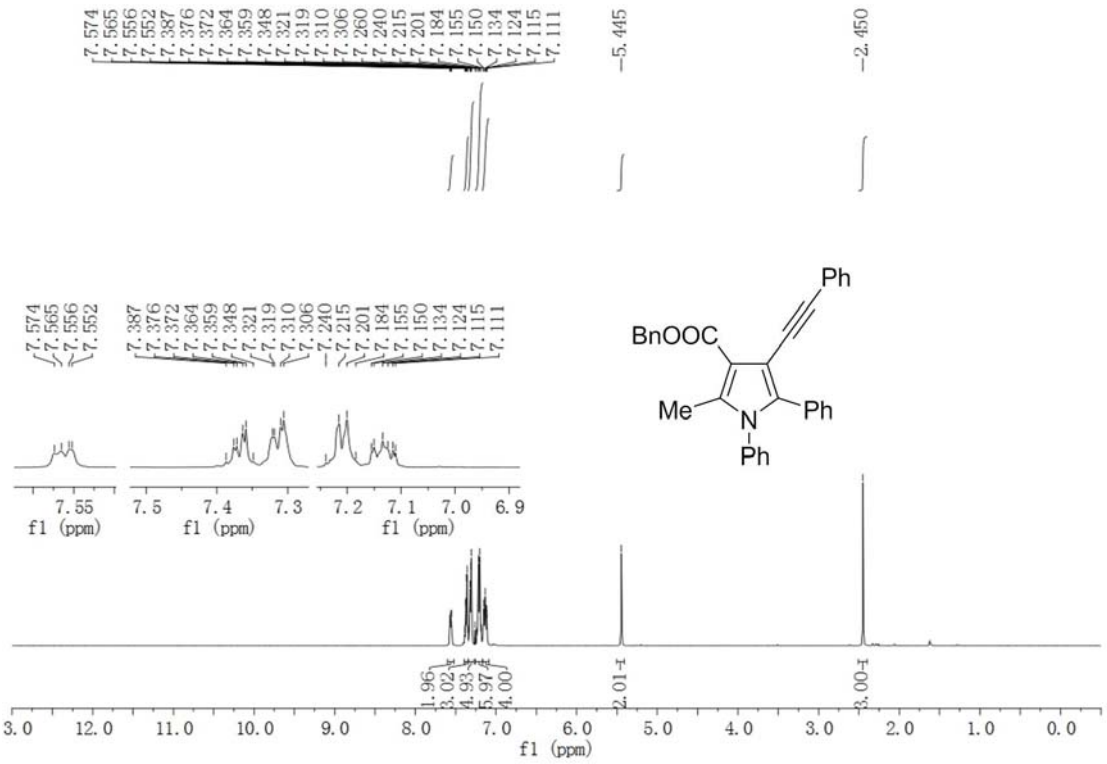
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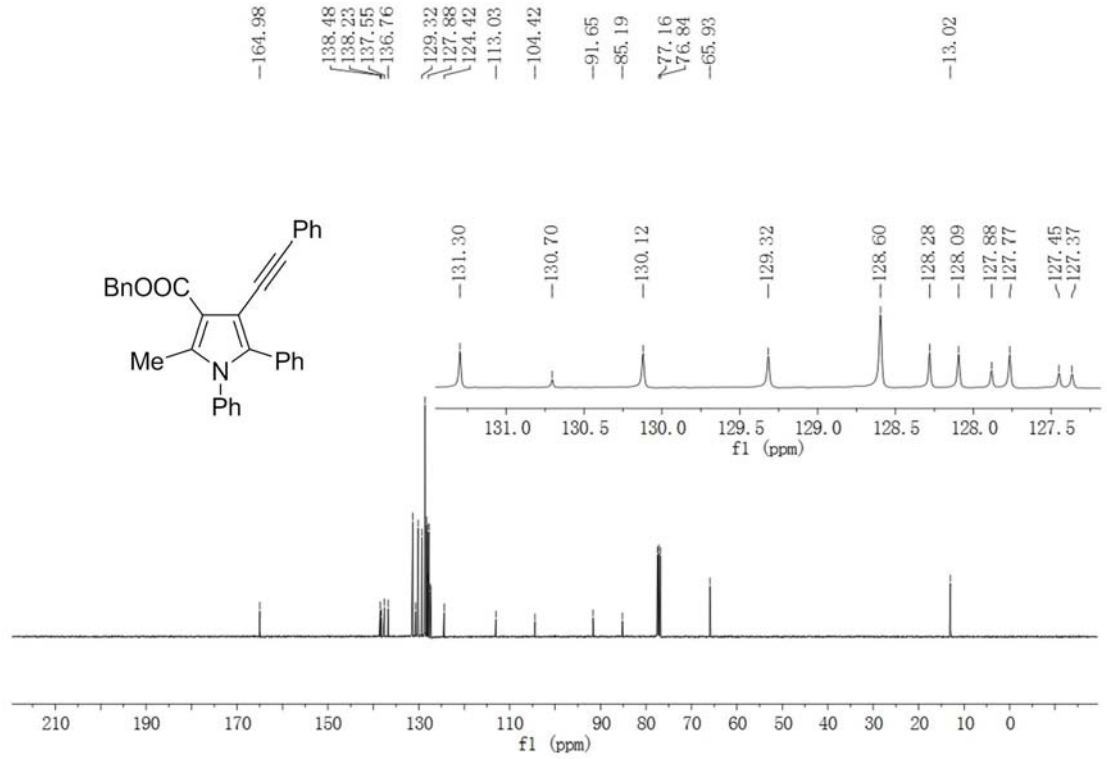
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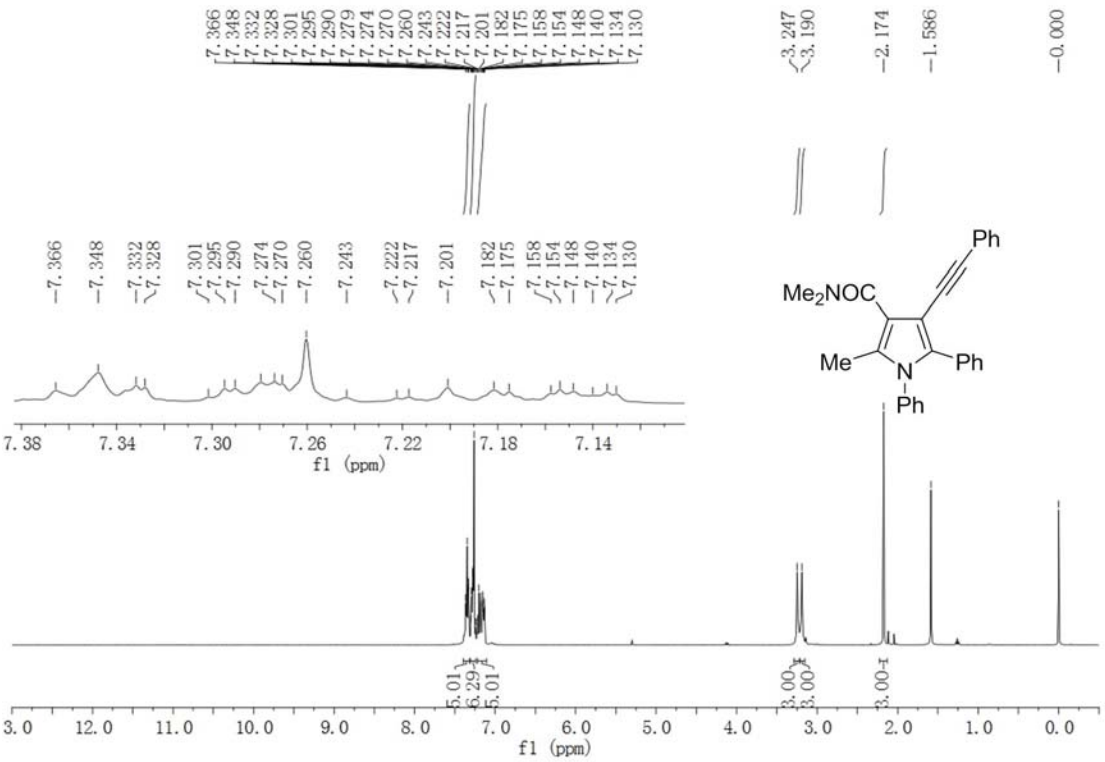
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7.260
7.243
7.222
7.217
7.201
7.182
7.175
7.158
7.154
7.148
7.140
7.134
7.130
3.247
3.190
2.174
1.586
0.000
Ph
Me2NOC
Me
N
Ph
Ph
7.38
7.34
7.30
7.26
7.22
7.18
7.14
f1 (ppm)
5.01
6.29
5.01
3.00
3.00
3.00
3.0
12.0
11.0
10.0
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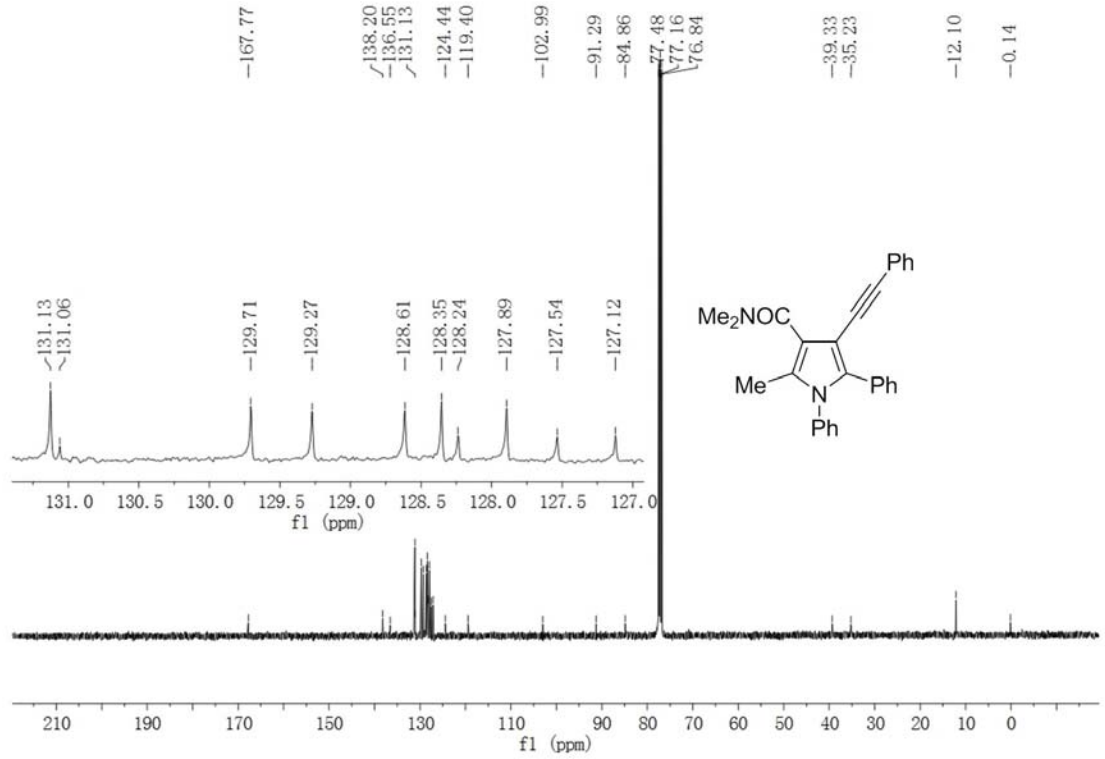
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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119.40
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91.29
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77.16
76.84
39.33
35.23
12.10
0.14
131.13
131.06
129.71
129.27
128.61
128.35
128.24
127.89
127.54
127.12
Ph
Me2NOC
Me
N
Ph
Ph
131.0
130.5
130.0
129.5
129.0
128.5
128.0
127.5
127.0
f1 (ppm)
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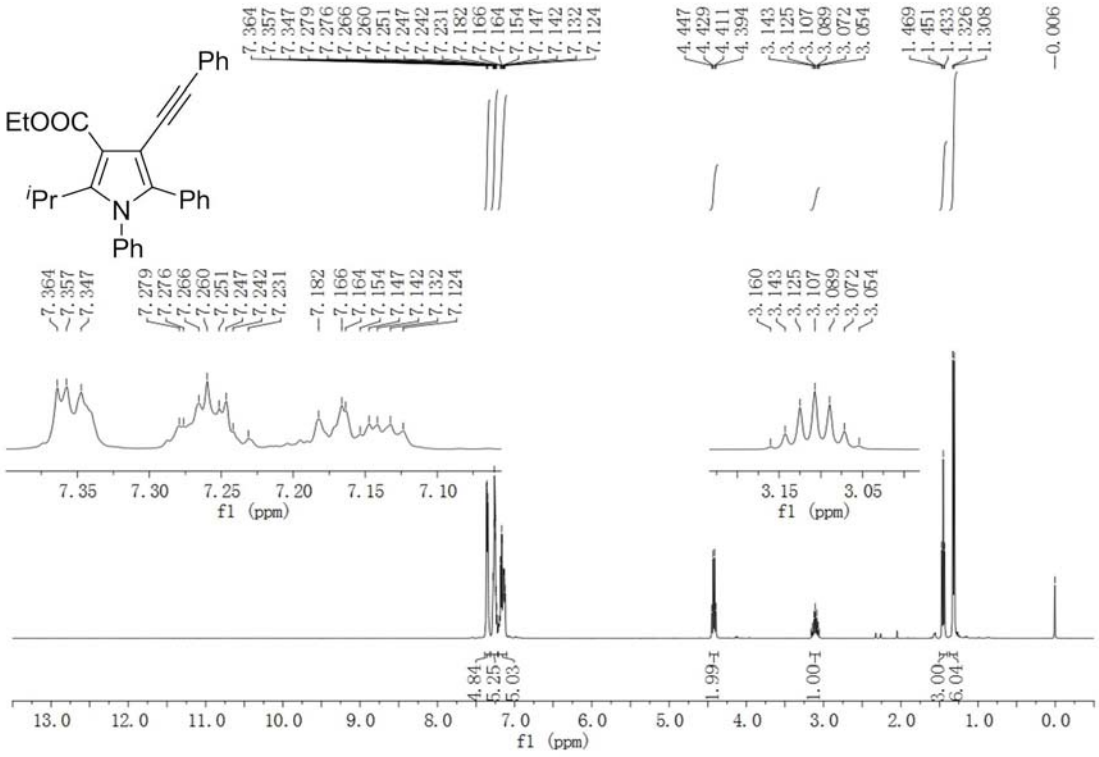
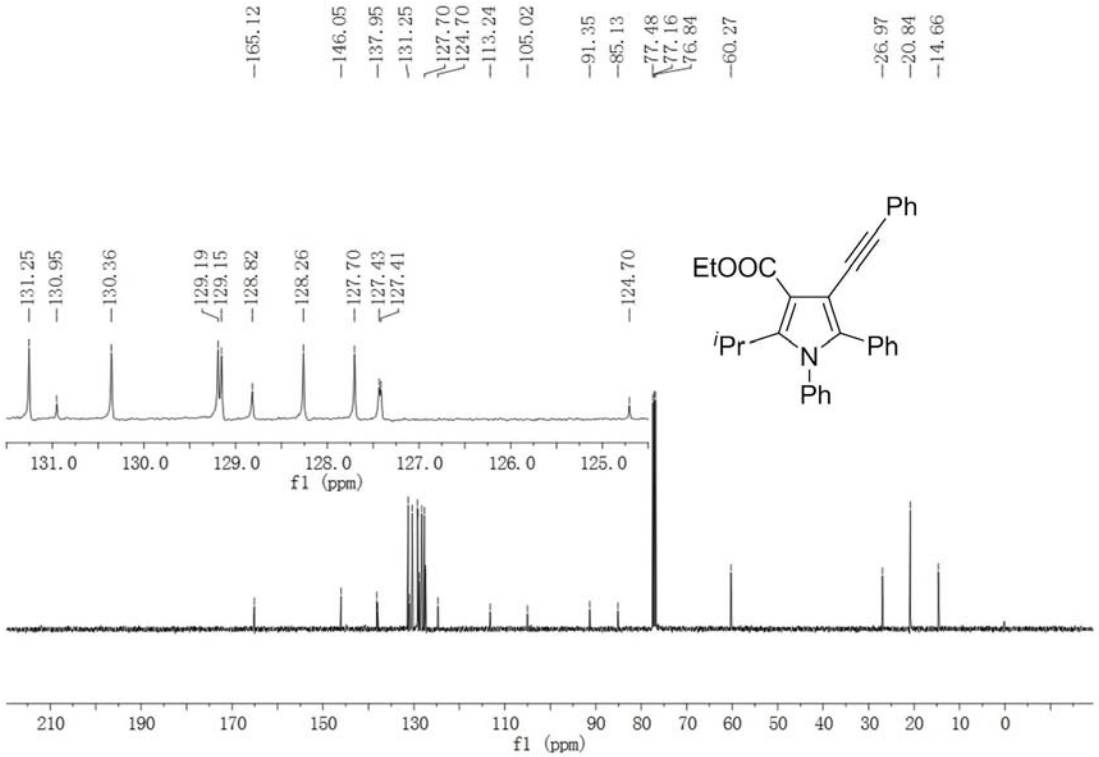
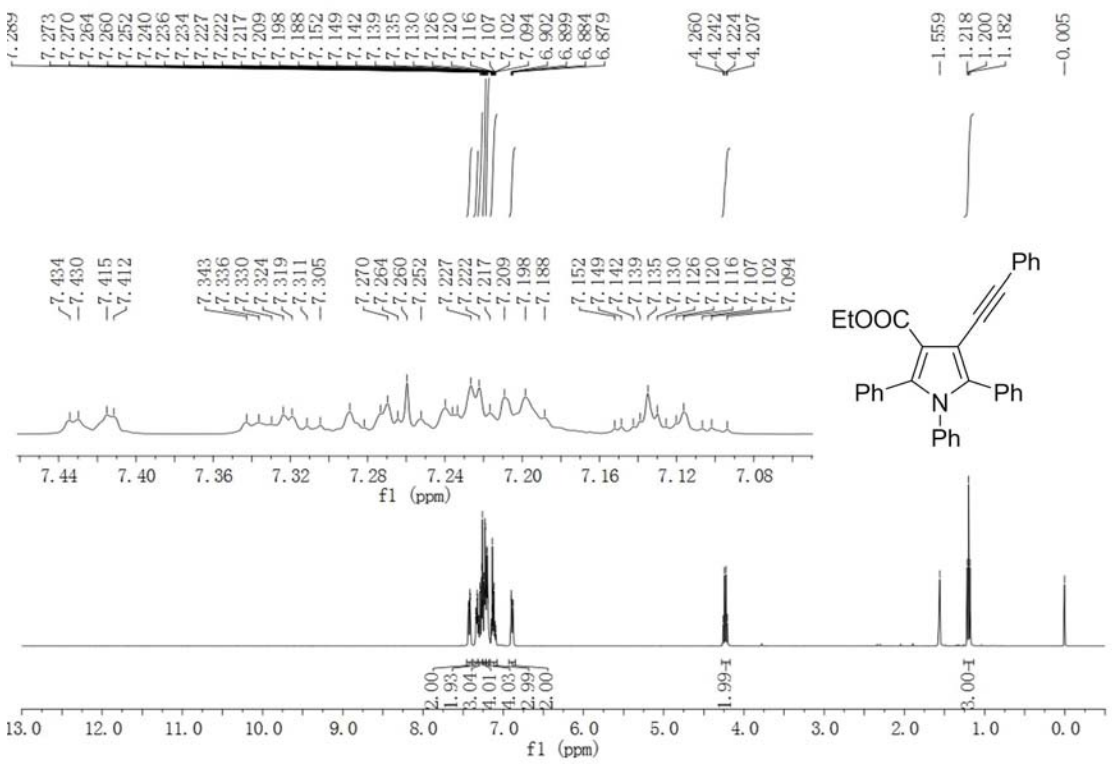
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Ph
EtOOC
iPr
N
Ph
Ph
f1 (ppm)


Ph
EtOOC
iPr
N
Ph
Ph
f1 (ppm)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7.236
7.234
7.227
7.222
7.217
7.209
7.198
7.188
7.152
7.149
7.142
7.139
7.135
7.130
7.126
7.120
7.116
7.107
7.102
7.094
6.902
6.899
6.884
6.879
4.260
4.242
4.224
4.207
1.559
1.218
1.200
1.182
0.005
7.434
7.430
7.415
7.412
7.343
7.336
7.330
7.324
7.319
7.311
7.305
7.270
7.264
7.260
7.252
7.227
7.222
7.217
7.209
7.198
7.188
7.152
7.149
7.142
7.139
7.135
7.130
7.126
7.120
7.116
7.107
7.102
7.094
Ph
EtOOC
Ph
Ph
N
Ph
7.44
7.40
7.36
7.32
7.28
7.24
7.20
7.16
7.12
7.08
f1 (ppm)
2.00
1.93
3.04
4.01
4.03
2.99
2.00
1.99
3.00
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12.0
11.0
10.0
9.0
8.0
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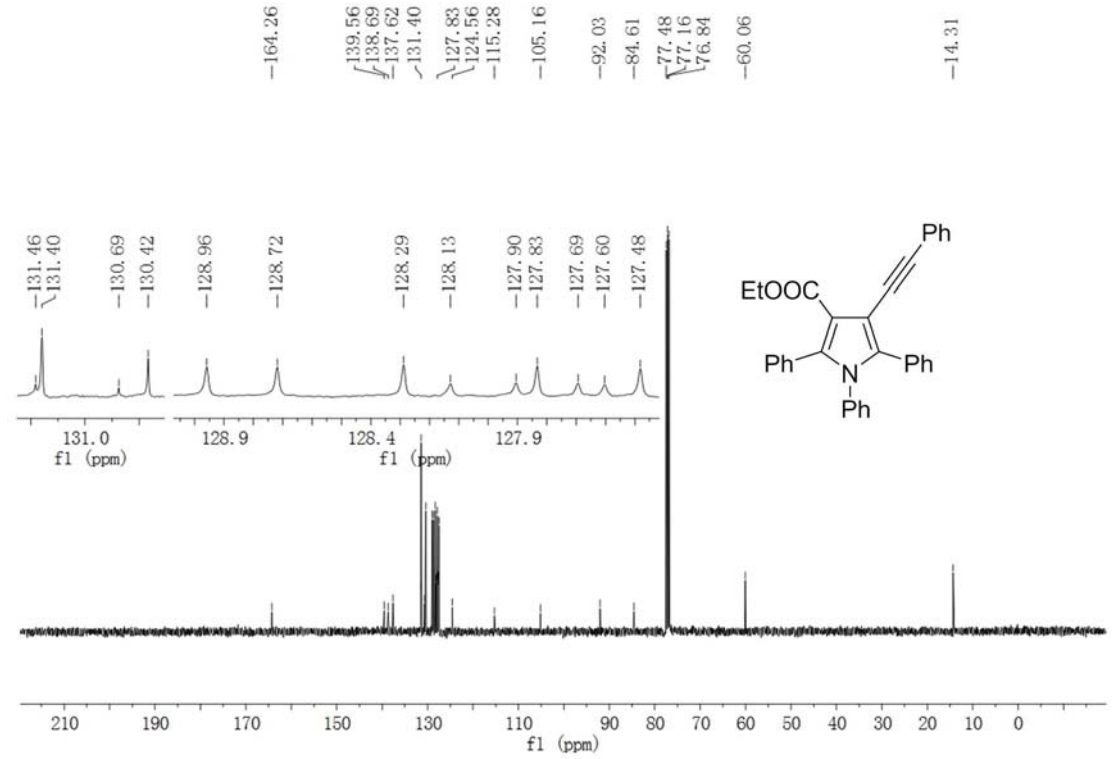
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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127.83
124.56
115.28
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92.03
84.61
77.48
77.16
76.84
60.06
14.31
131.46
131.40
130.69
130.42
128.96
128.72
128.29
128.13
127.90
127.83
127.69
127.60
127.48
Ph
EtOOC
Ph
Ph
N
Ph
131.0
f1 (ppm)
128.9
128.4
f1 (ppm)
127.9
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170
150
130
110
90
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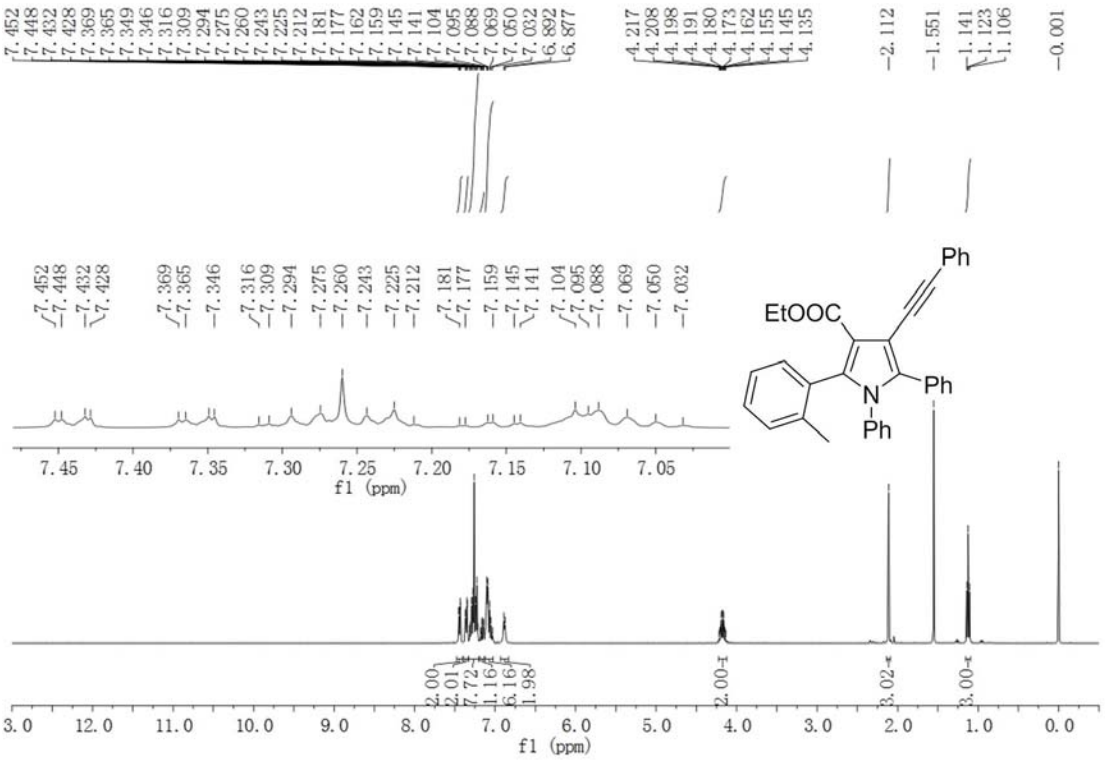
50
40
30
20
10
0
f1 (ppm)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7.346
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7.309
7.294
7.275
7.260
7.243
7.225
7.212
7.181
7.177
7.162
7.159
7.145
7.141
7.104
7.095
7.088
7.069
7.050
7.032
6.892
6.877
4.217
4.208
4.198
4.191
4.180
4.173
4.162
4.155
4.145
4.135
2.112
1.551
1.141
1.123
1.106
0.001
EtOOC
Ph
N
Ph
Ph
f1 (ppm)
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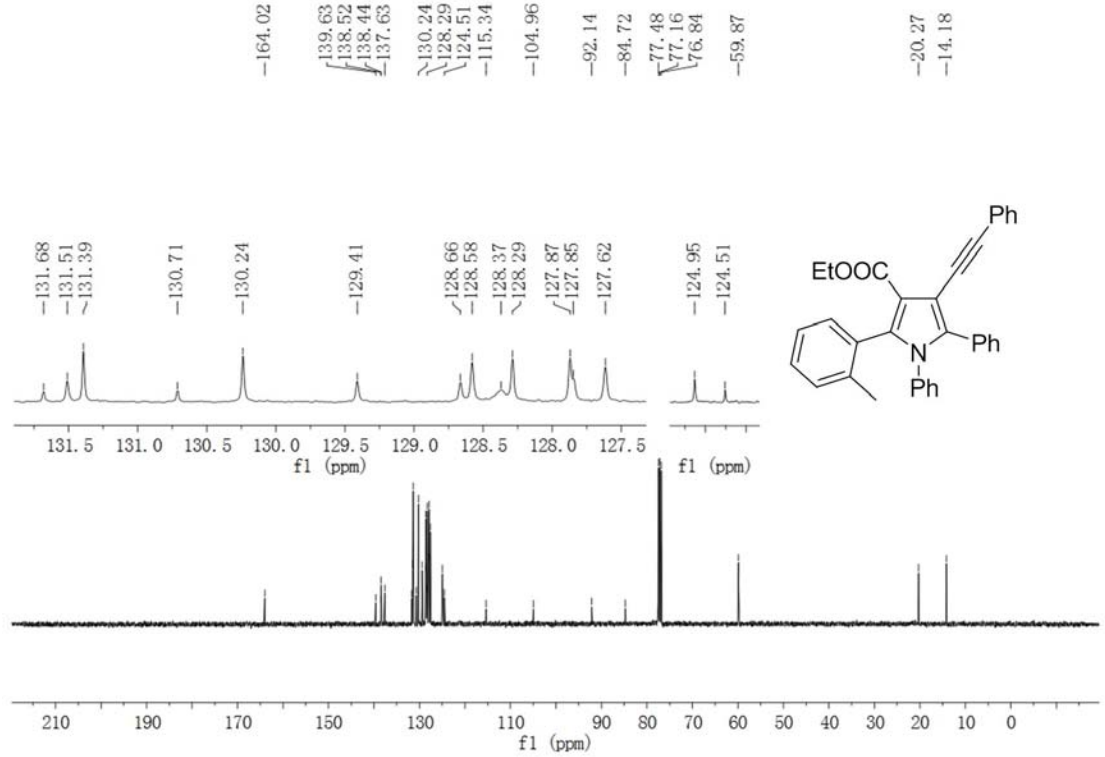
2.01
7.72
1.16
6.16
1.98
2.00
3.02
3.00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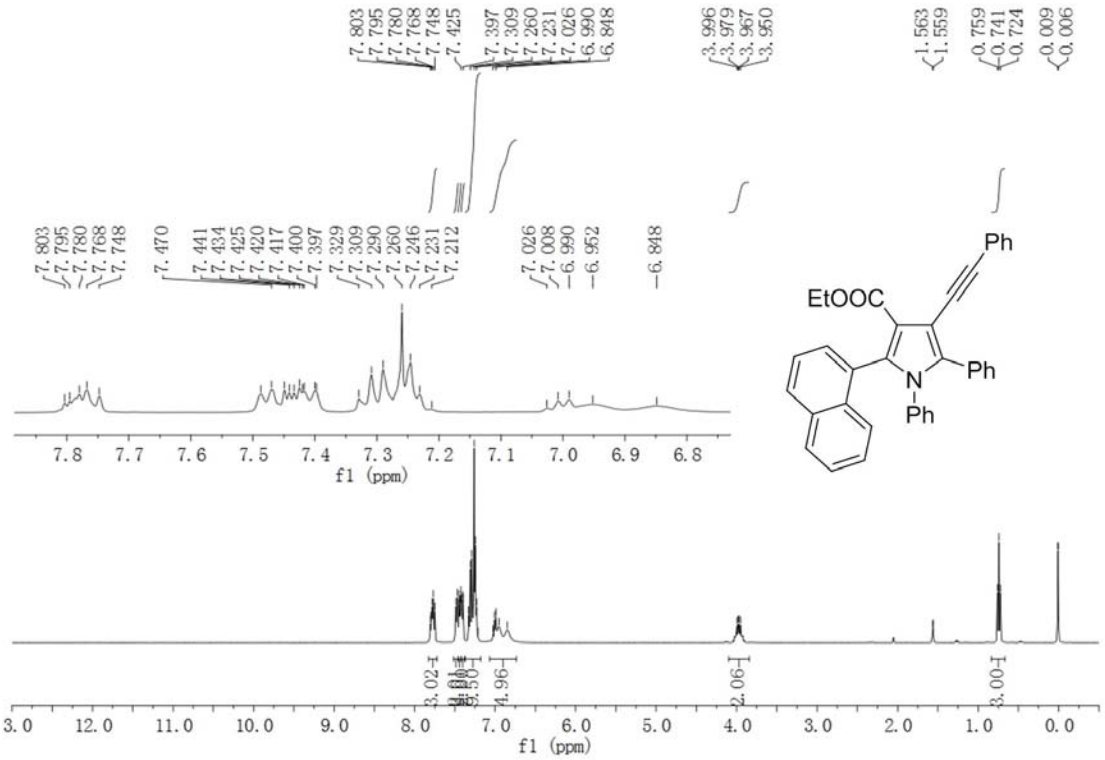
130.24
128.29
124.51
115.34
104.96
92.14
84.72
77.48
77.16
76.84
59.87
20.27
14.18
131.68
131.51
131.39
130.71
130.24
129.41
128.66
128.58
128.37
128.29
127.87
127.85
127.62
124.95
124.51
EtOOC
Ph
N
Ph
Ph
f1 (ppm)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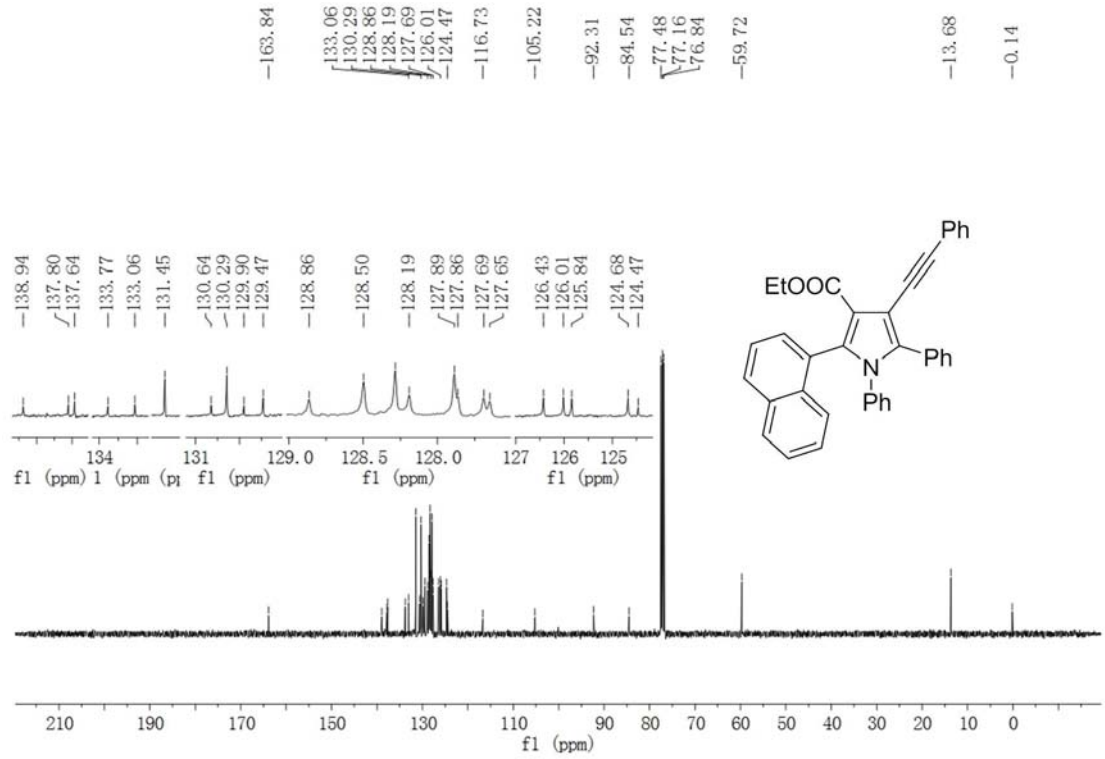
7.780
7.768
7.748
7.425
7.397
7.309
7.260
7.231
7.026
6.990
6.848
3.996
3.979
3.967
3.950
1.563
1.559
0.759
0.741
0.724
0.009
0.006
7.470
7.441
7.434
7.425
7.420
7.417
7.400
7.397
7.329
7.309
7.290
7.260
7.246
7.231
7.212
7.026
7.008
6.990
6.952
6.848
Ph
EtOOC
Ph
N
Ph
f1 (ppm)
3.02
4.96
2.06
3.00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128.19
127.69
126.01
124.47
116.73
105.22
92.31
84.54
77.48
77.16
76.84
59.72
13.68
0.14
138.94
137.80
137.64
133.77
133.06
131.45
130.64
130.29
129.90
129.47
128.86
128.50
128.19
127.89
127.86
127.69
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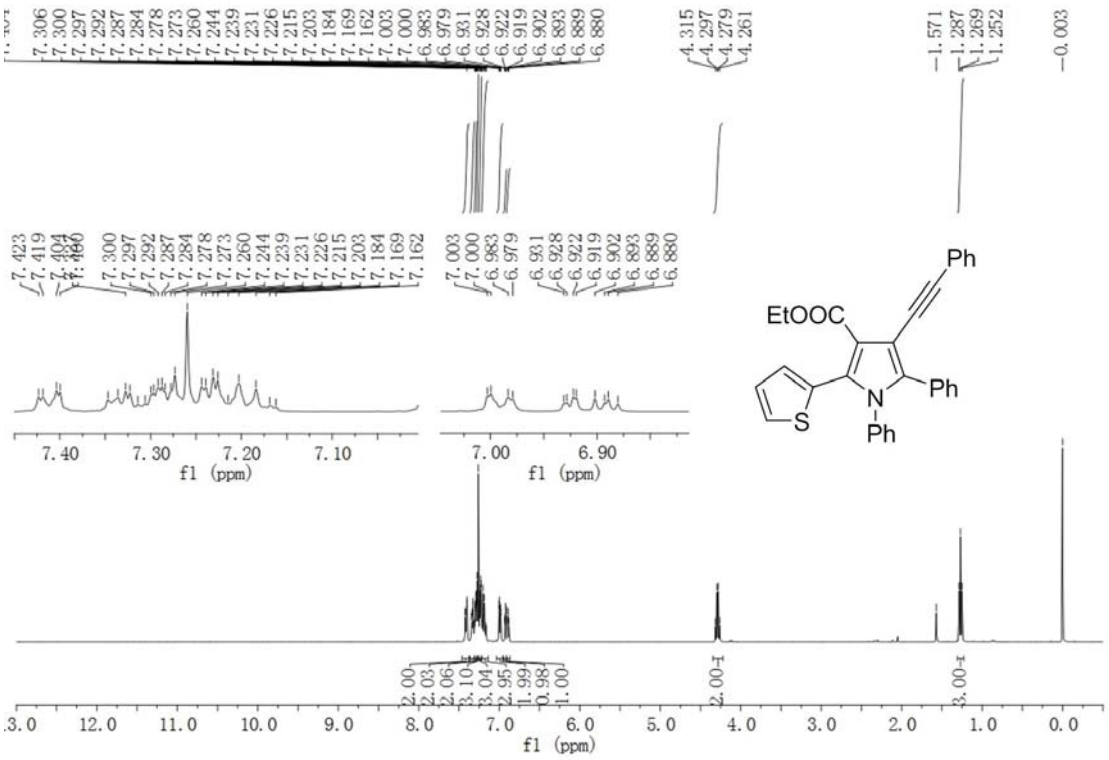
126.43
126.01
125.84
124.68
124.47
Ph
EtOOC
Ph
N
Ph
f1 (ppm)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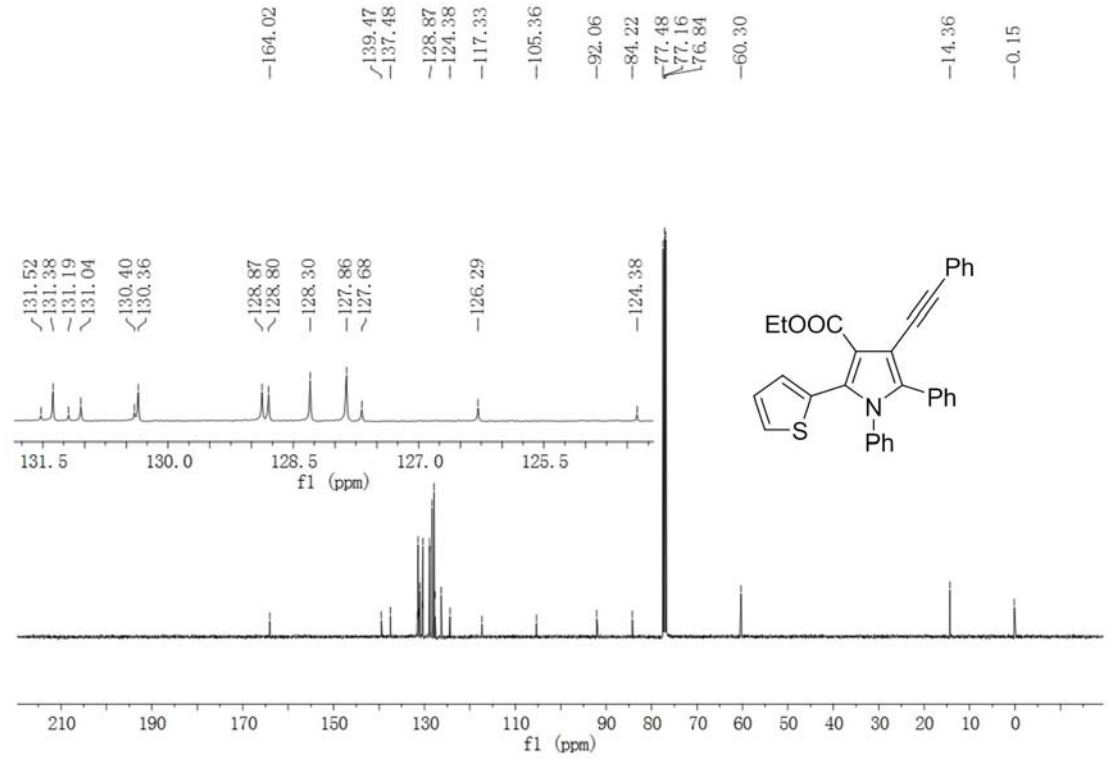
7.297
7.292
7.287
7.284
7.278
7.273
7.260
7.244
7.239
7.231
7.226
7.215
7.203
7.184
7.169
7.162
7.003
7.000
6.983
6.979
6.931
6.928
6.922
6.919
6.902
6.893
6.889
6.880
4.315
4.297
4.279
4.261
1.571
1.287
1.269
1.252
0.003
7.423
7.419
7.404
7.300
7.297
7.292
7.287
7.284
7.278
7.273
7.260
7.244
7.239
7.231
7.226
7.215
7.203
7.184
7.169
7.162
7.003
7.000
6.983
6.979
6.931
6.928
6.922
6.919
6.902
6.893
6.889
6.880
7.40
7.30
7.20
7.10
f1 (ppm)
7.00
6.90
f1 (ppm)
Ph
EtOOC
Ph
N
Ph
S
2.00
2.03
2.06
3.10
3.04
2.95
1.99
0.98
1.00
2.00
3.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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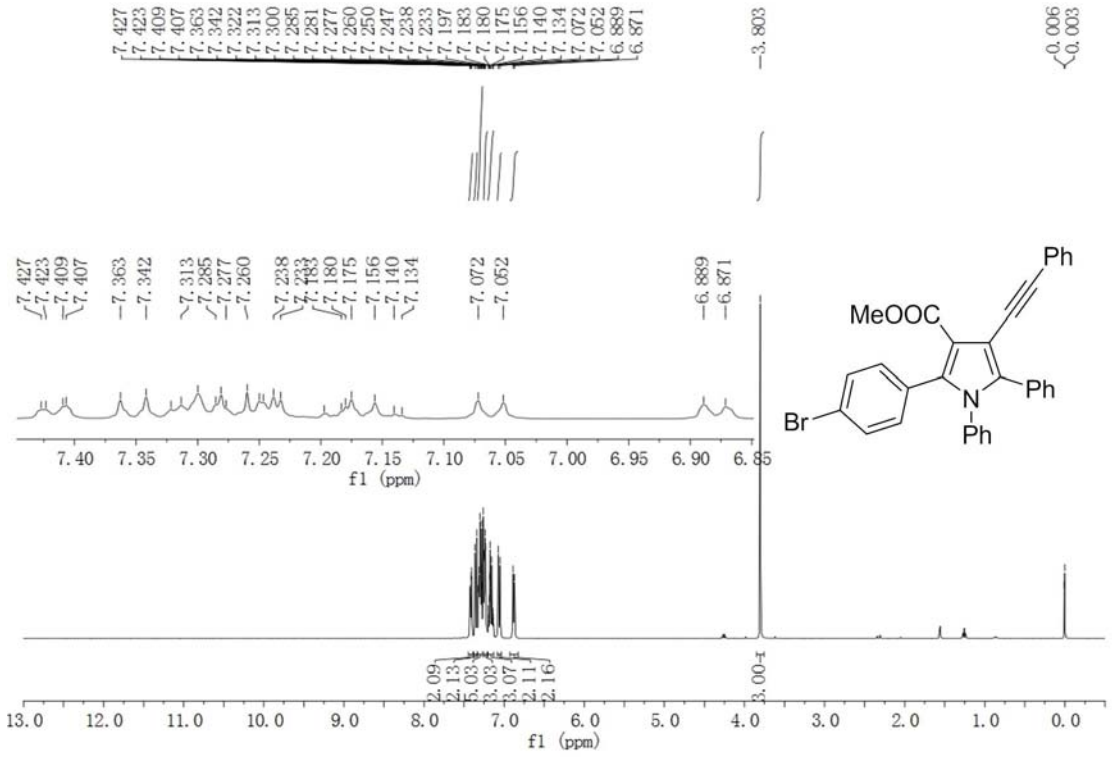
117.33
105.36
92.06
84.22
77.48
77.16
76.84
60.30
14.36
0.15
131.52
131.38
131.19
131.04
130.40
130.36
128.87
128.80
128.30
127.86
127.68
126.29
124.38
131.5
130.0
128.5
127.0
125.5
f1 (ppm)
Ph
EtOOC
Ph
N
Ph
S
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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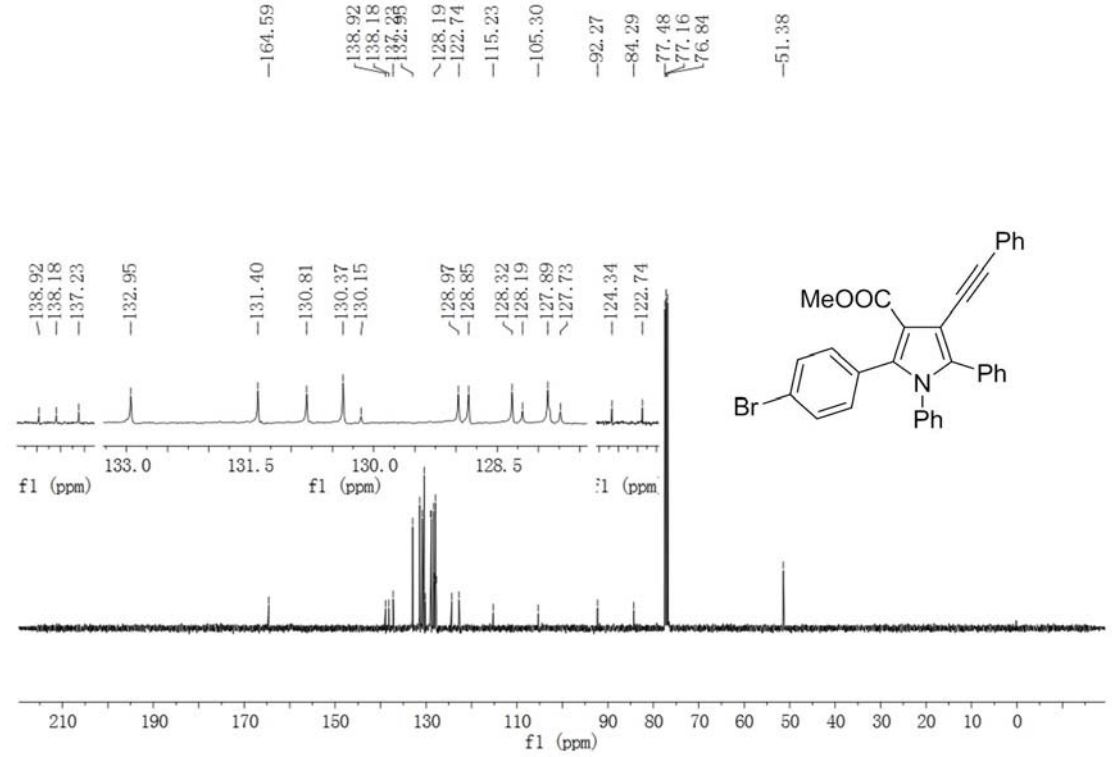
7.313
7.300
7.285
7.281
7.277
7.260
7.250
7.247
7.238
7.233
7.197
7.183
7.180
7.175
7.156
7.140
7.134
7.072
7.052
6.889
6.871
3.803
0.006
0.003
MeOOC
Ph
Ph
N
Ph
Br
f1 (ppm)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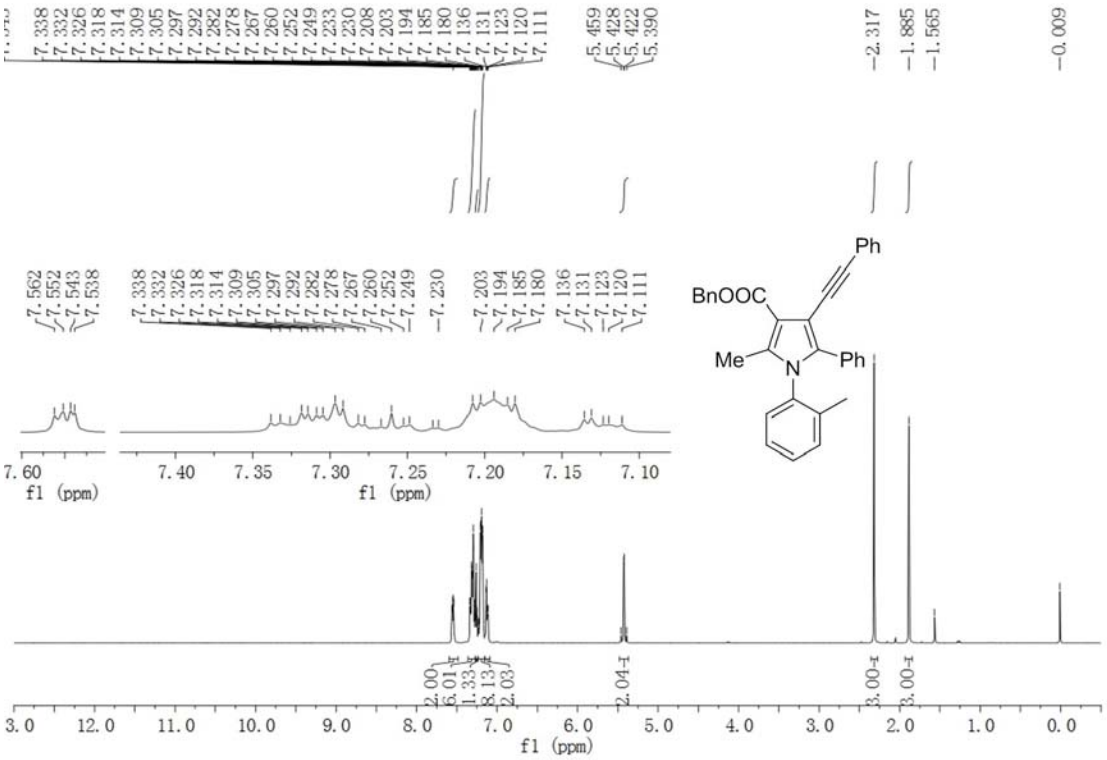
138.18
137.23
132.95
128.19
122.74
115.23
105.30
92.27
84.29
77.48
77.16
76.84
51.38
MeOOC
Ph
Ph
N
Ph
Br
f1 (ppm)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7.260
7.252
7.249
7.233
7.230
7.208
7.203
7.194
7.185
7.180
7.136
7.131
7.123
7.120
7.111
5.459
5.428
5.422
5.390
2.317
1.885
1.565
0.009
7.562
7.552
7.543
7.538
Ph
BnOOC
Me
N
Ph
f1 (ppm)
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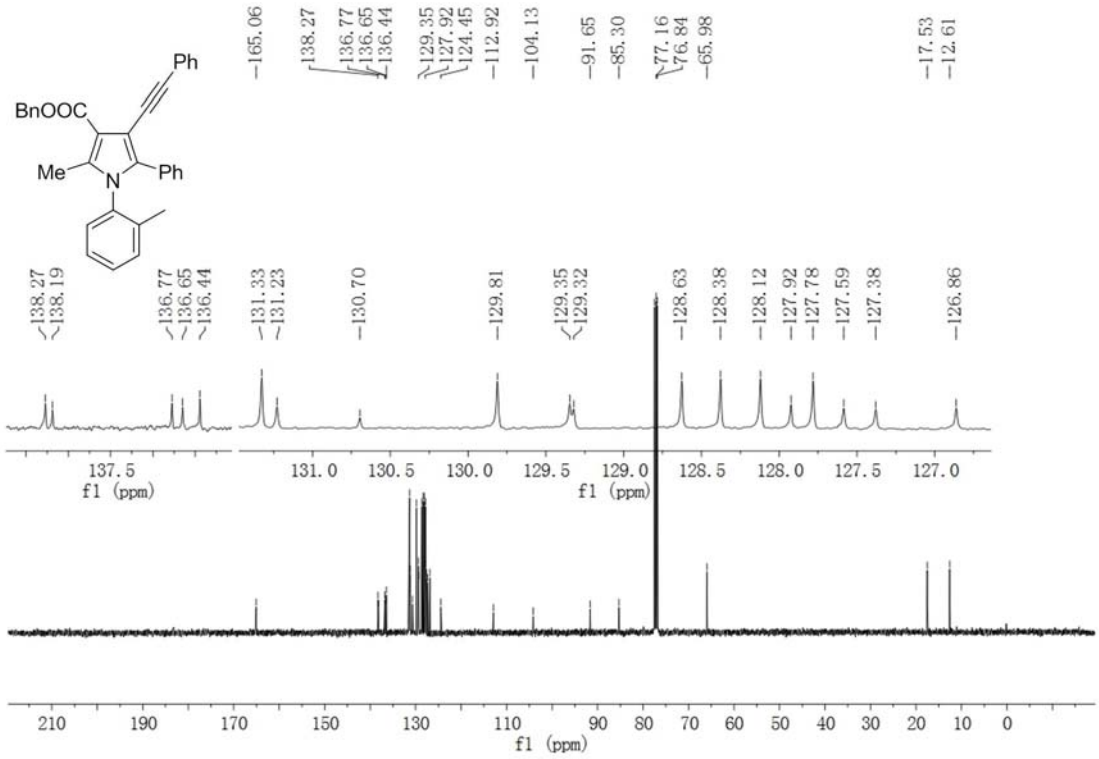
6.01
1.33
8.13
2.03
2.04
3.00
3.00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124.45
112.92
104.13
91.65
85.30
77.16
76.84
65.98
17.53
12.61
Ph
BnOOC
Me
N
Ph
138.27
138.19
136.77
136.65
136.44
131.33
131.23
130.70
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128.63
128.38
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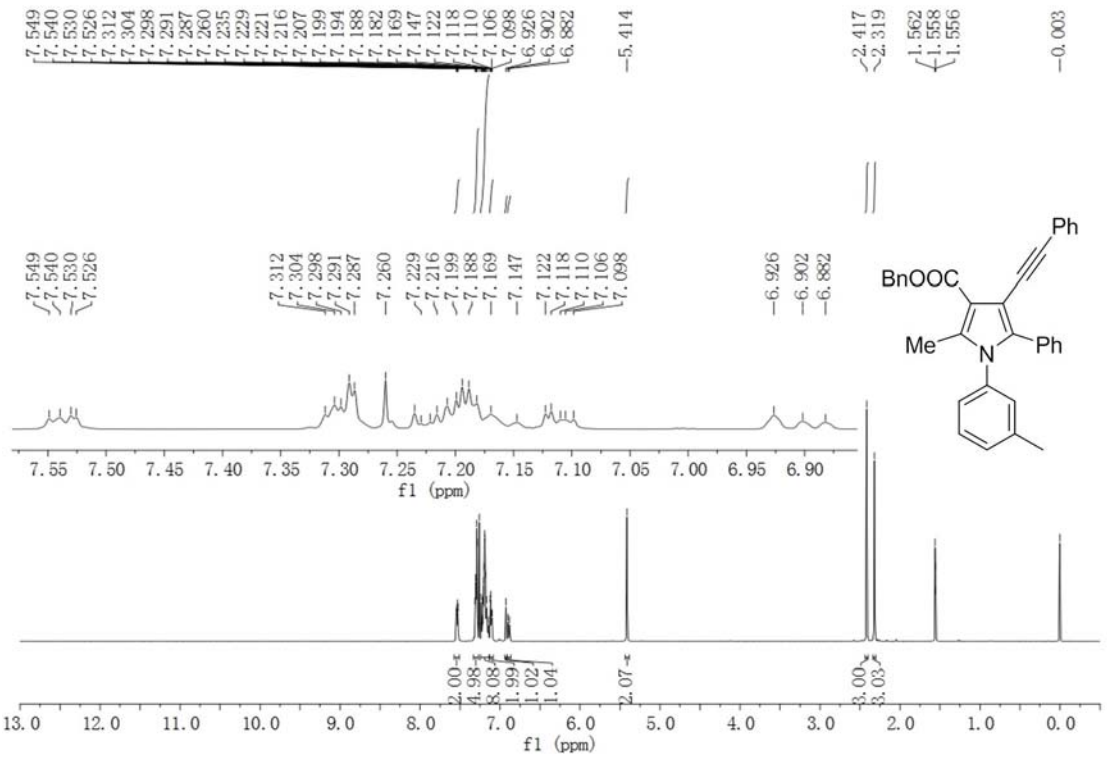
127.59
127.38
126.86
f1 (ppm)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7.312
7.304
7.298
7.291
7.287
7.260
7.235
7.229
7.221
7.216
7.207
7.199
7.194
7.188
7.182
7.169
7.147
7.122
7.118
7.110
7.106
7.098
6.926
6.902
6.882
5.414
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2.319
1.562
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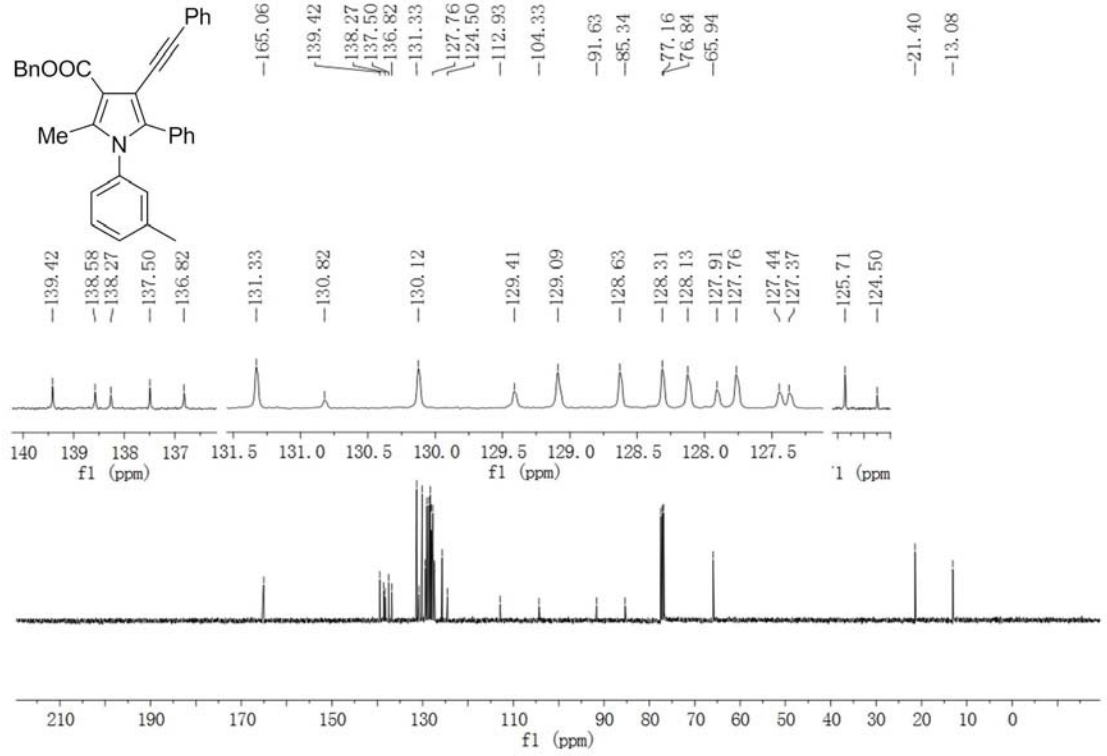
BnOOC
Ph
Me
N
Ph
f1 (ppm)


BnOOC
Ph
Me
N
Ph
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138.27
137.50
136.82
131.33
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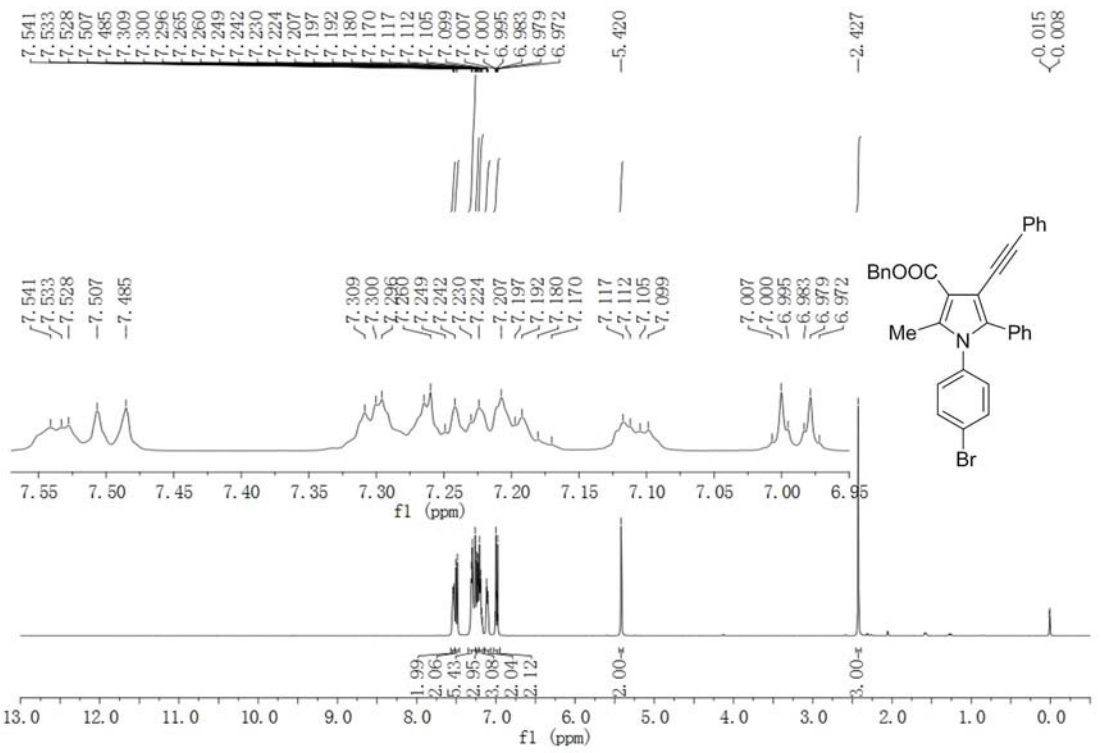
104.33
91.63
85.34
77.16
76.84
65.94
21.40
13.08
f1 (ppm)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7.296
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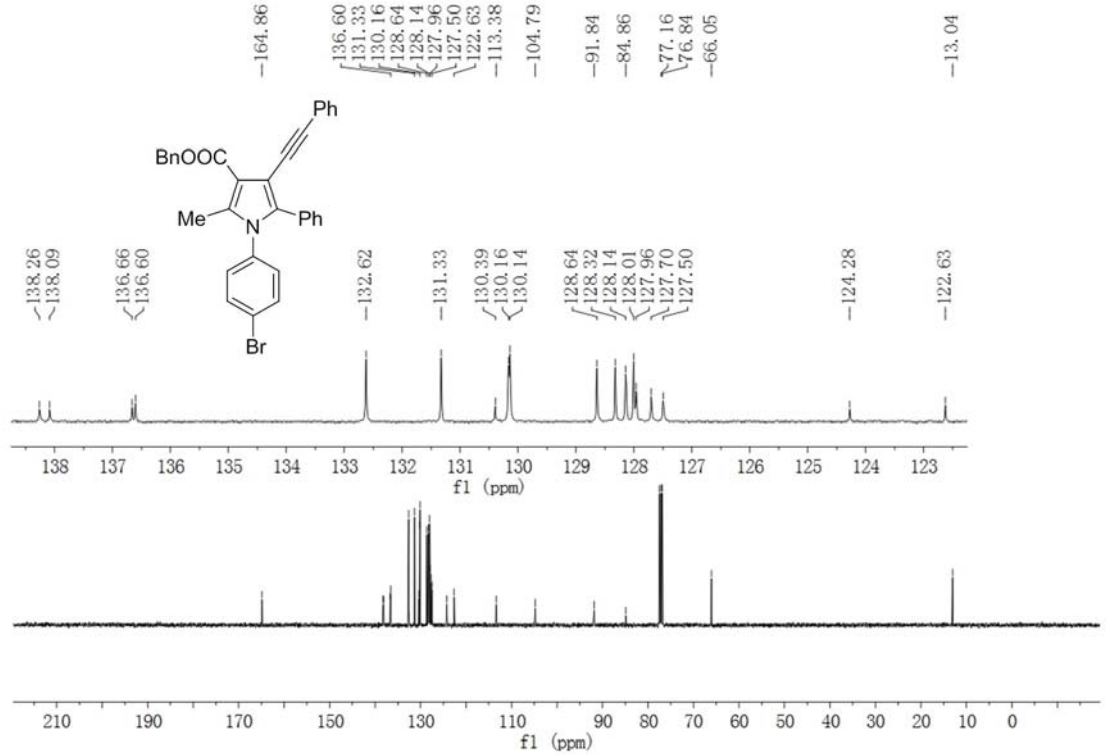
7.260
7.249
7.242
7.230
7.224
7.207
7.197
7.192
7.180
7.170
7.117
7.112
7.105
7.099
7.007
7.000
6.995
6.983
6.979
6.972
5.420
2.427
0.015
0.008
Ph
BnOOC
Me
N
Ph
Br
7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95
f1 (ppm)
1.99
1.06
5.43
2.95
3.08
2.04
2.12
2.00
3.00
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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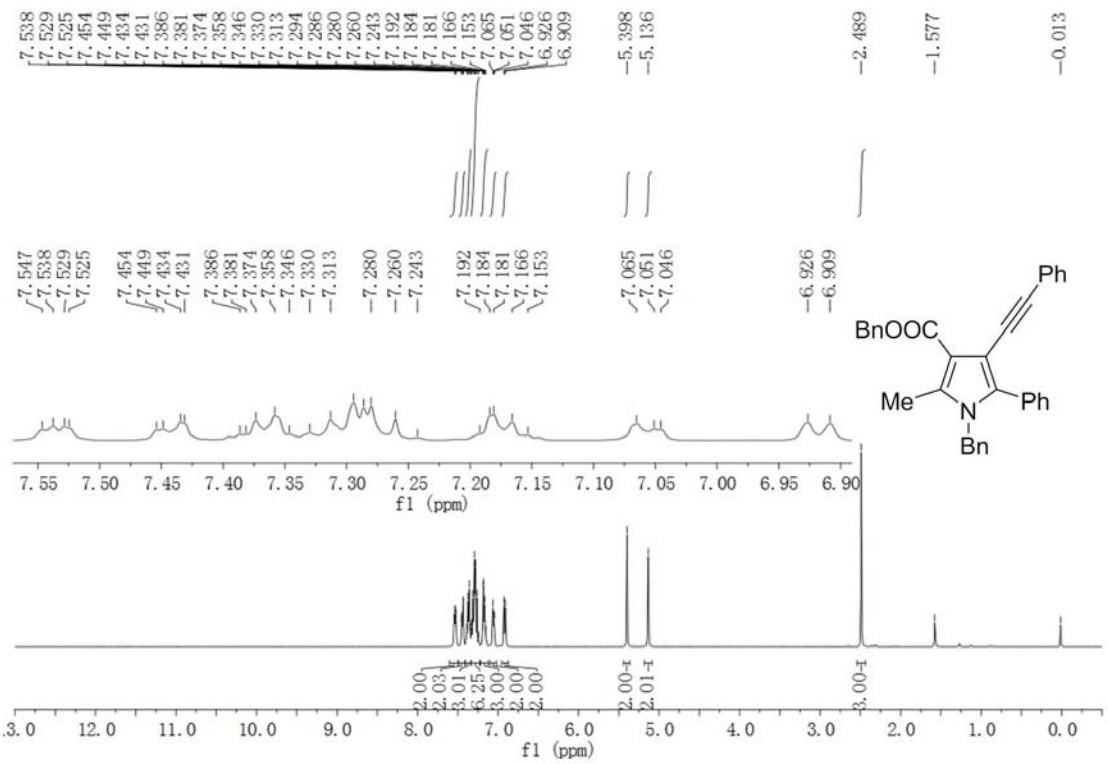
127.50
122.63
113.38
104.79
91.84
84.86
77.16
76.84
66.05
13.04
Ph
BnOOC
Me
N
Ph
Br
138.26
138.09
136.66
136.60
132.62
131.33
130.39
130.16
130.14
128.64
128.32
128.14
128.01
127.96
127.70
127.50
124.28
122.63
138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.358
7.346
7.330
7.313
7.294
7.286
7.280
7.260
7.243
7.192
7.184
7.181
7.166
7.153
7.065
7.051
7.046
6.926
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5.136
2.489
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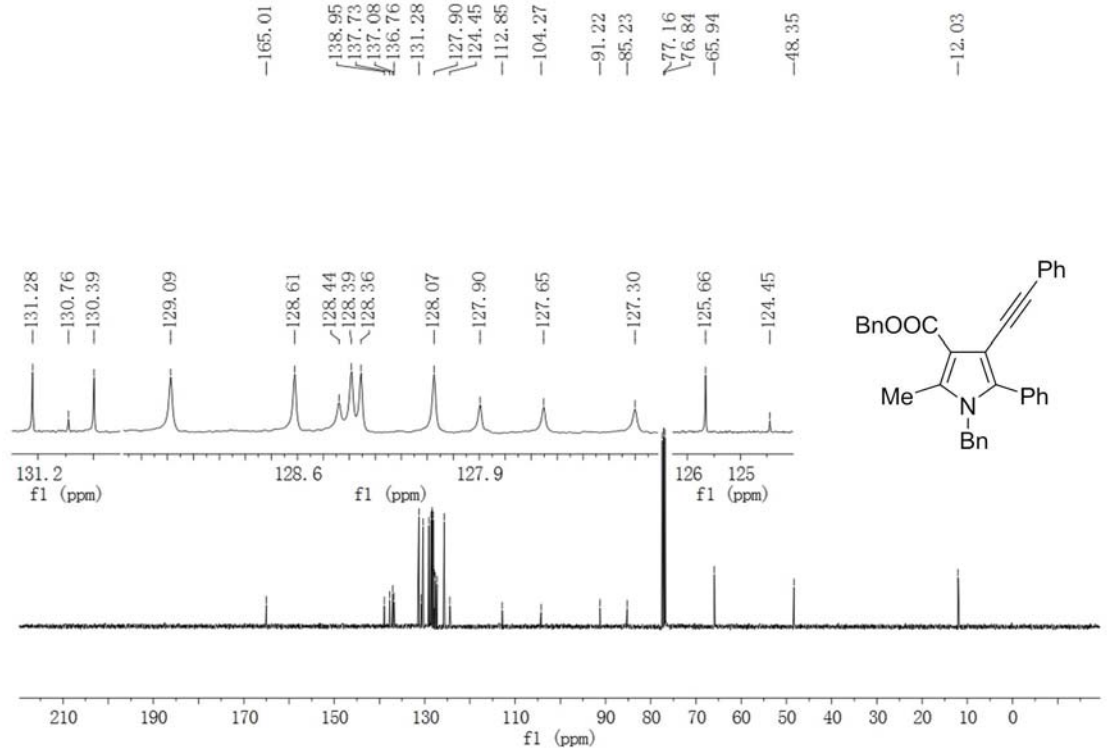
Ph
BnOOC
Me
N
Ph
Bn
f1 (ppm)


165.01
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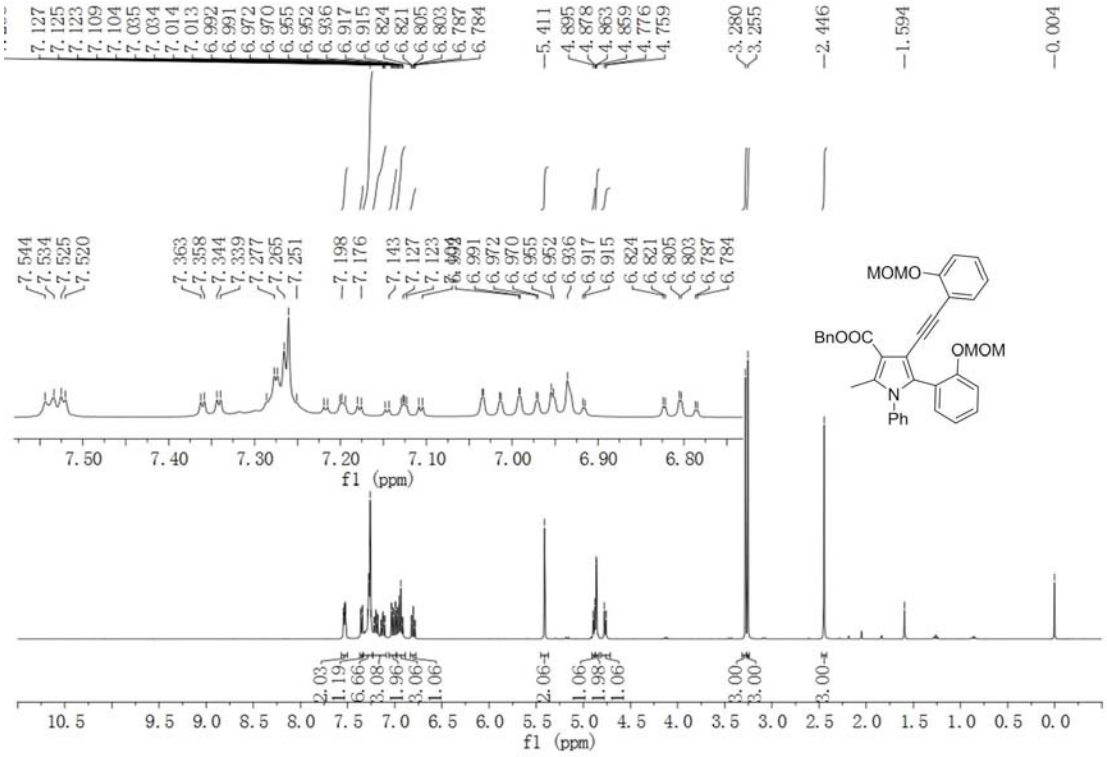
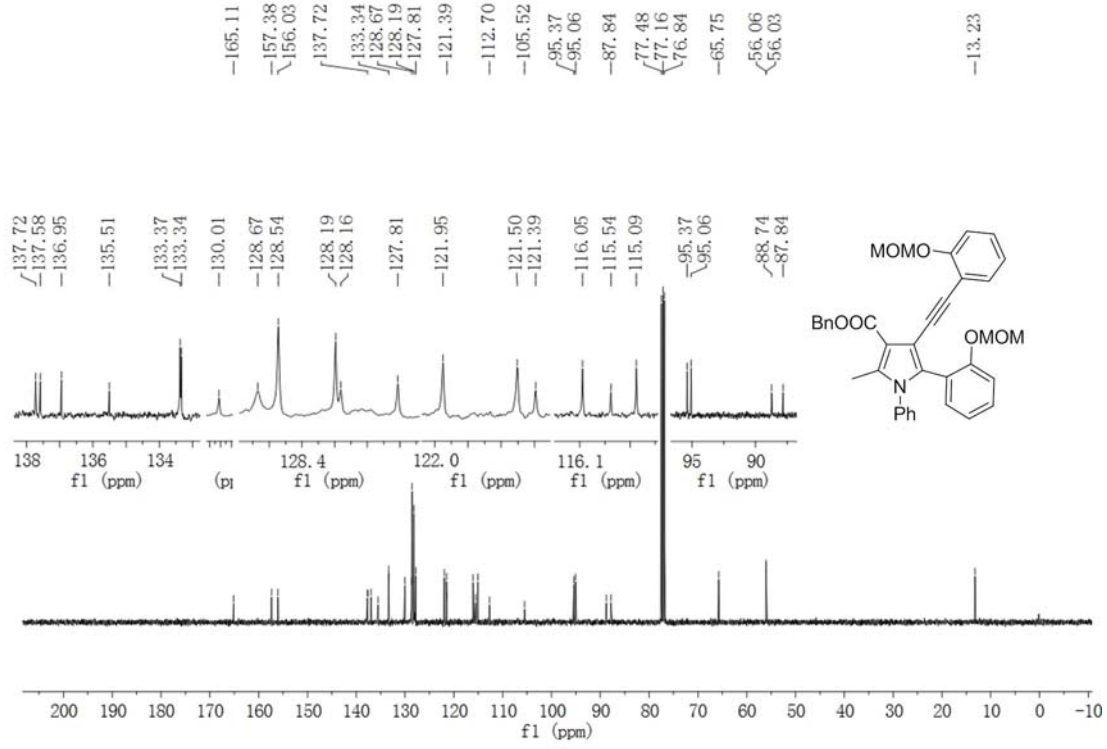
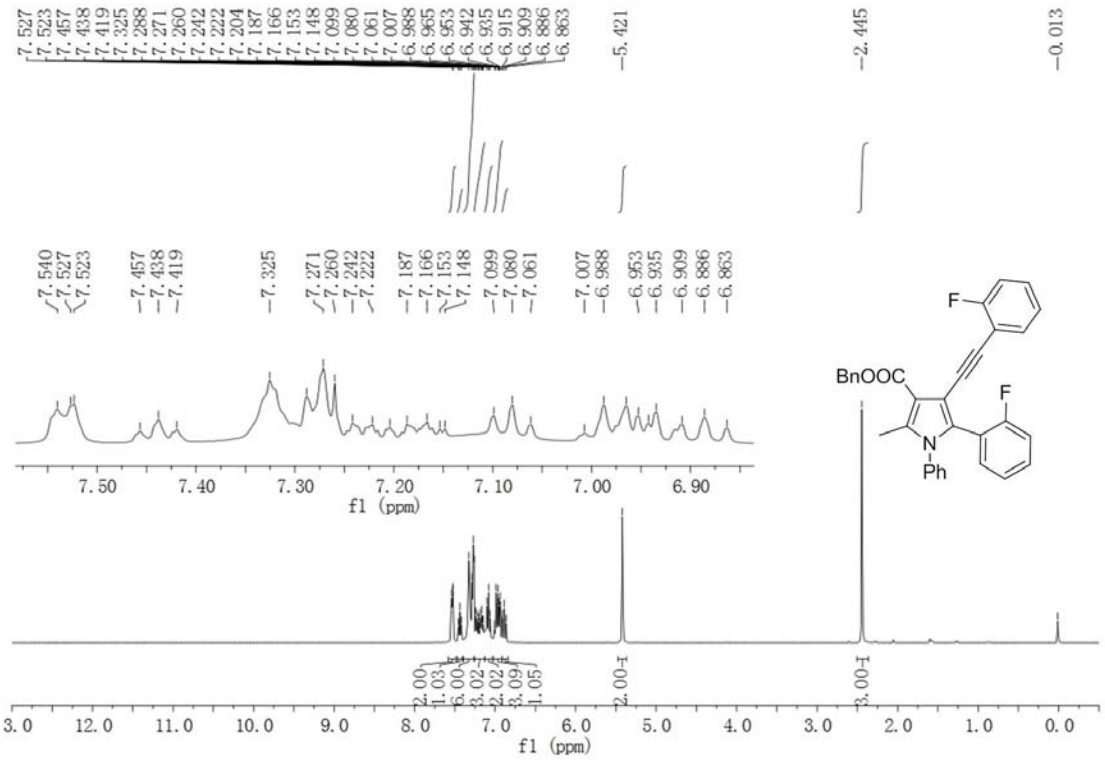
137.08
136.76
131.28
127.90
124.45
112.85
104.27
91.22
85.23
77.16
76.84
65.94
48.35
12.03
Ph
BnOOC
Me
N
Ph
Bn
f1 (ppm)


MOMO
BnOOC
OMOM
N
Ph
f1 (ppm)


MOMO
BnOOC
OMOM
N
Ph
f1 (ppm)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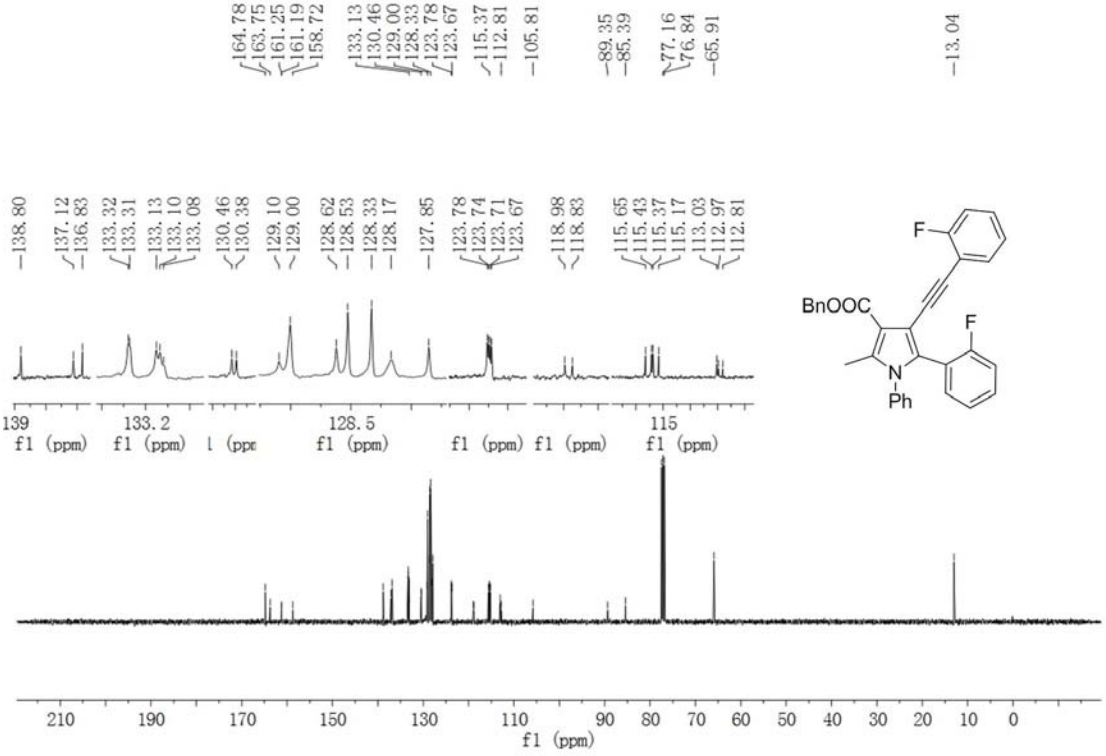
7.457
7.438
7.419
7.325
7.288
7.271
7.260
7.242
7.222
7.204
7.187
7.166
7.153
7.148
7.099
7.080
7.061
7.007
6.988
6.965
6.953
6.942
6.935
6.915
6.909
6.886
6.863
5.421
2.445
0.013
7.50
7.40
7.30
7.20
7.10
7.00
6.90
f1 (ppm)
BnOOC
F
F
N
Ph
2.00
1.03
6.00
3.02
2.02
3.09
1.05
2.00
3.00
3.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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158.72
133.13
130.46
129.00
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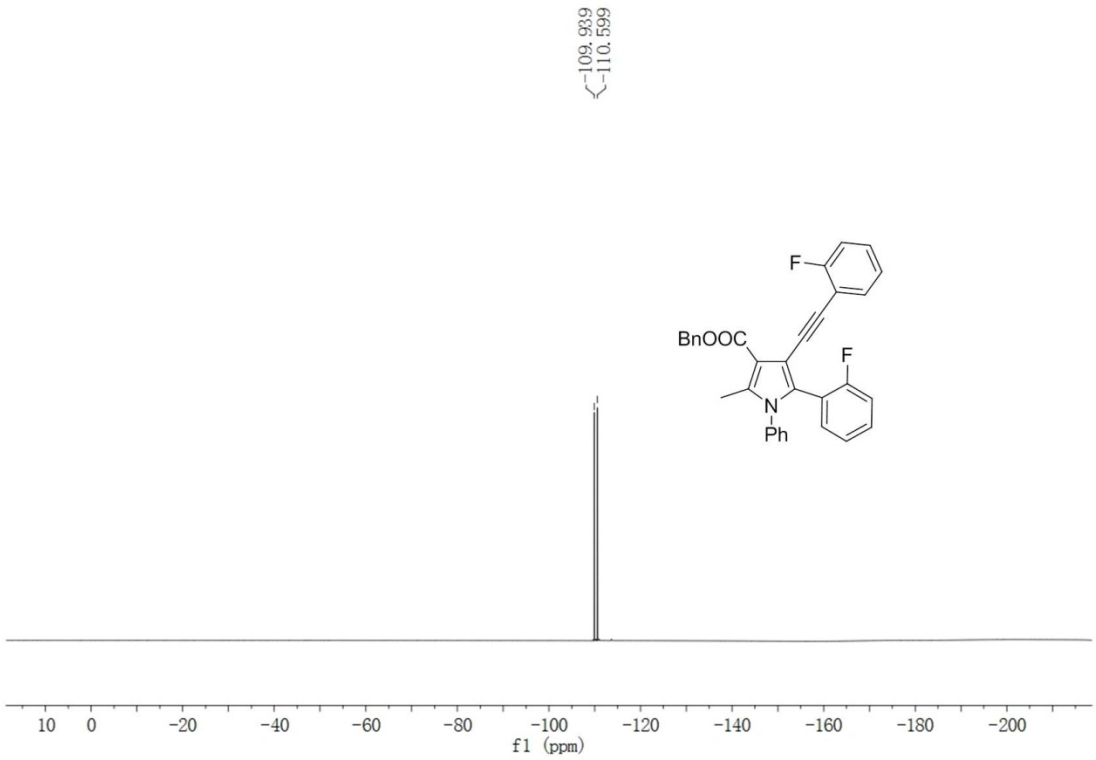
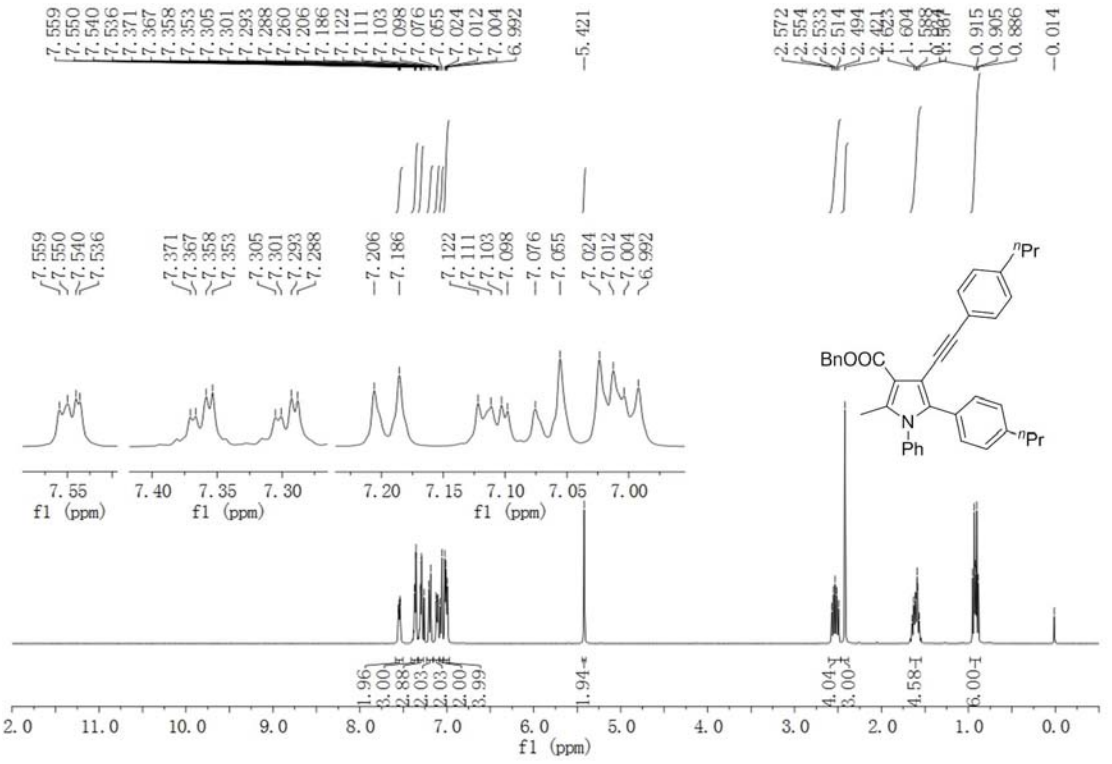
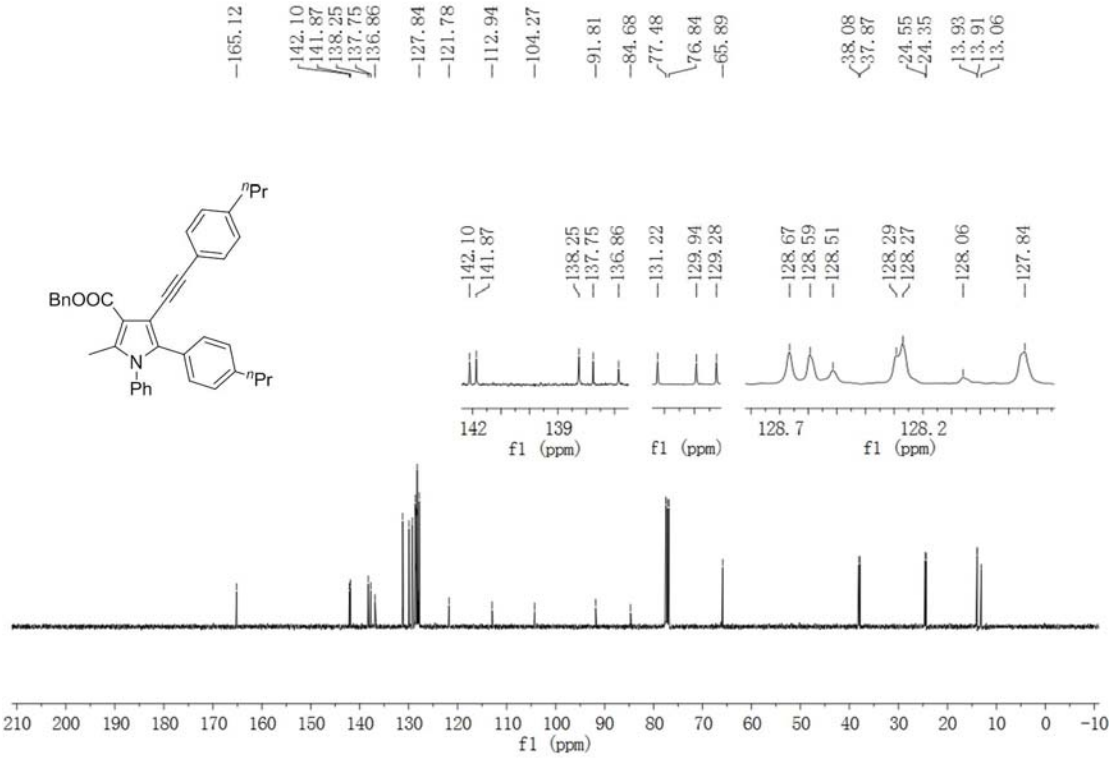
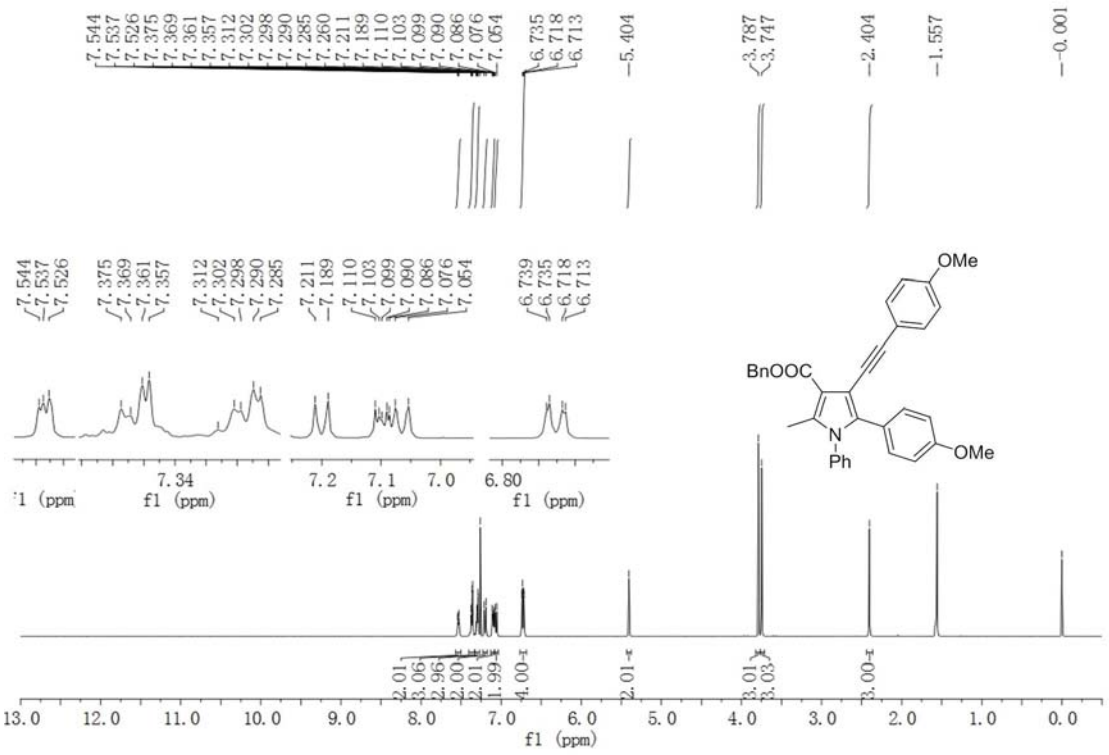
123.78
123.67
115.37
112.81
105.81
89.35
85.39
77.16
76.84
65.91
13.04
138.80
137.12
136.83
133.32
133.31
133.13
133.10
133.08
130.46
130.38
129.10
129.00
128.62
128.53
128.33
128.17
127.85
123.78
123.74
123.71
123.67
118.98
118.83
115.65
115.43
115.37
115.17
113.03
112.97
112.81
139
133.2
128.5
115
f1 (ppm)
BnOOC
F
F
N
Ph
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-109.939
-110.599
F
BnOOC
F
N
Ph
10
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)


BnOOC
nPr
N
Ph
f1 (ppm)


BnOOC
nPr
N
Ph
f1 (ppm)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7.312
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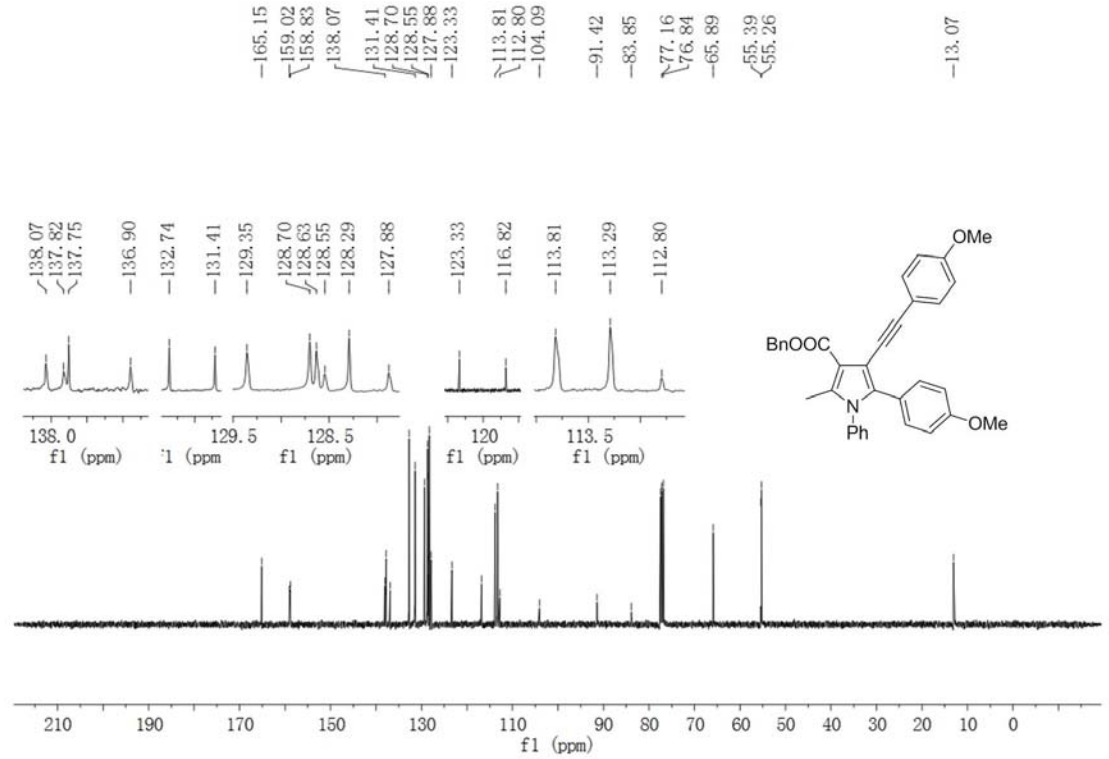
7.298
7.290
7.285
7.260
7.211
7.189
7.110
7.103
7.099
7.090
7.086
7.076
7.054
6.735
6.718
6.713
5.404
3.787
3.747
2.404
1.557
0.001
OMe
BnOOC
N
Ph
OMe
f1 (ppm)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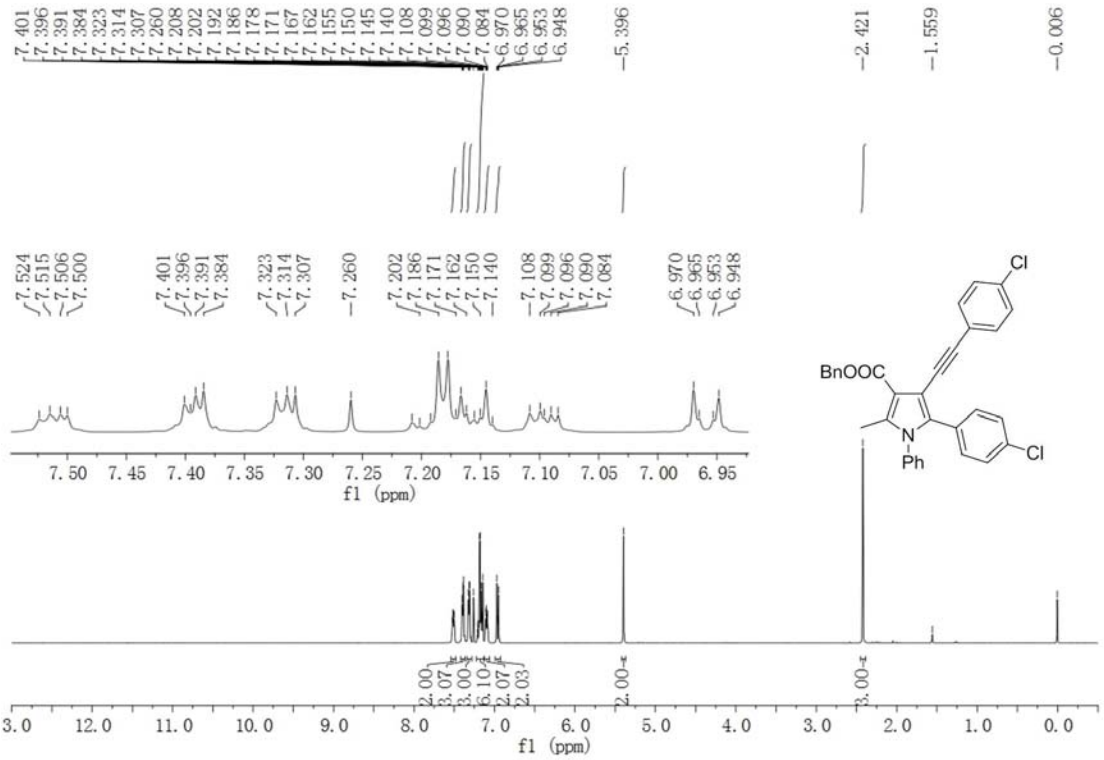
159.02
158.83
138.07
131.41
128.70
128.55
127.88
123.33
113.81
112.80
104.09
91.42
83.85
77.16
76.84
65.89
55.39
55.26
13.07
OMe
BnOOC
N
Ph
OMe
f1 (ppm)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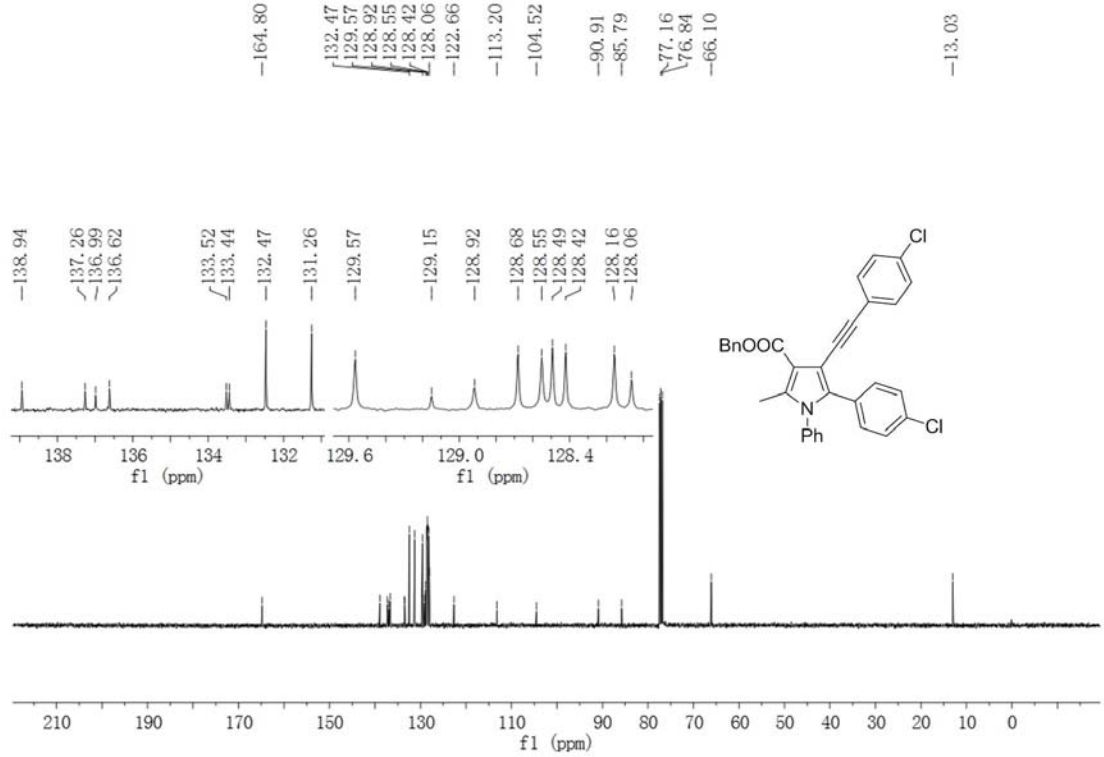
7.396
7.391
7.384
7.323
7.314
7.307
7.260
7.208
7.202
7.192
7.186
7.178
7.171
7.167
7.162
7.155
7.150
7.145
7.140
7.108
7.099
7.096
7.090
7.084
6.970
6.965
6.953
6.948
5.396
2.421
1.559
0.006
7.524
7.515
7.506
7.500
7.401
7.396
7.391
7.384
7.323
7.314
7.307
7.260
7.202
7.186
7.171
7.162
7.150
7.140
7.108
7.099
7.096
7.090
7.084
6.970
6.965
6.953
6.948
7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95
f1 (ppm)
Cl
BnOOC
N
Ph
Cl
2.00
3.07
3.00
6.10
2.07
2.03
2.00
3.00
3.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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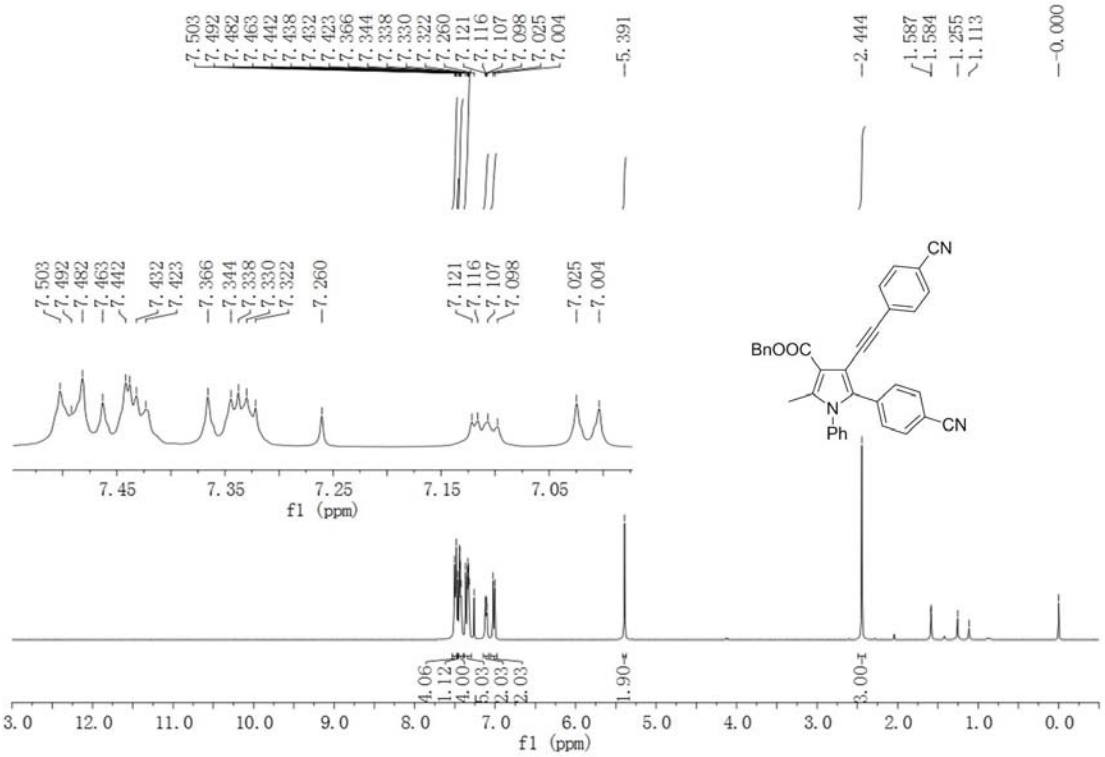
129.57
128.92
128.55
128.42
128.06
122.66
113.20
104.52
90.91
85.79
77.16
76.84
66.10
13.03
138.94
137.26
136.99
136.62
133.52
133.44
132.47
131.26
129.57
129.15
128.92
128.68
128.55
128.49
128.42
128.16
128.06
138 136 134 132
f1 (ppm)
129.6 129.0 128.4
f1 (ppm)
Cl
BnOOC
N
Ph
Cl
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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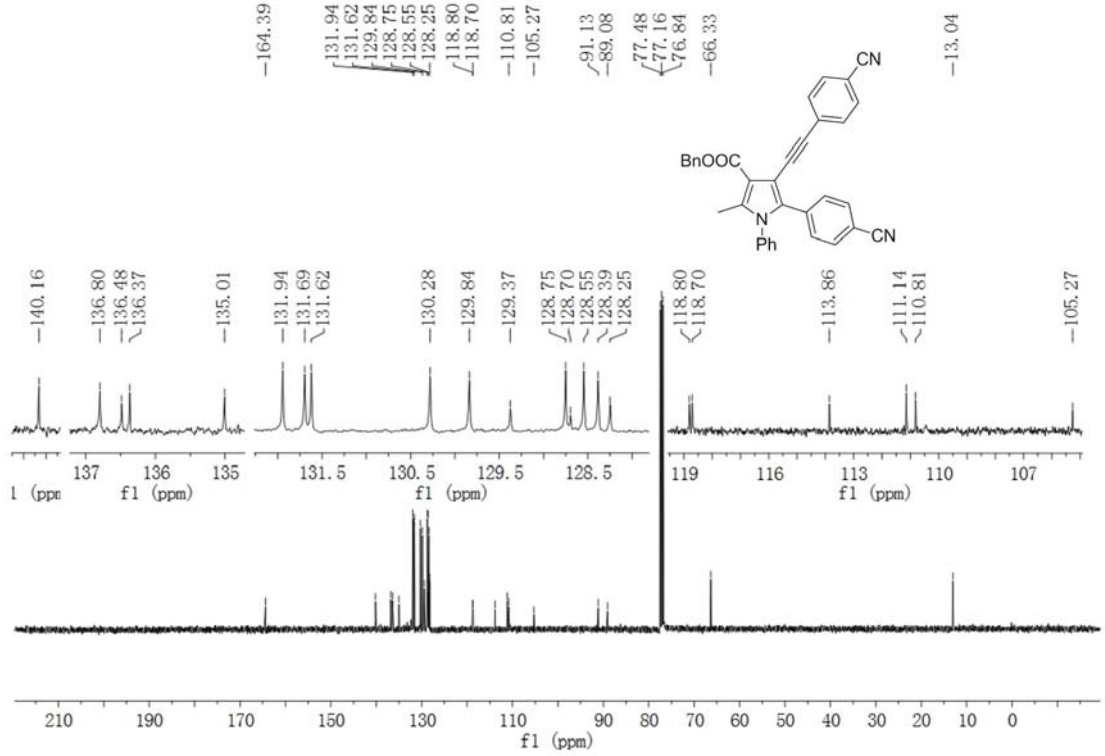
7.482
7.463
7.442
7.438
7.432
7.423
7.366
7.344
7.338
7.330
7.322
7.260
7.121
7.116
7.107
7.098
7.025
7.004
5.391
2.444
1.587
1.584
1.255
1.113
0.000
CN
BnOOC
N
Ph
CN
7.45
7.35
7.25
7.15
7.05
f1 (ppm)
4.06
1.12
4.00
5.03
2.03
2.03
1.90
3.00
3.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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128.55
128.25
118.80
118.70
110.81
105.27
91.13
89.08
77.48
77.16
76.84
66.33
13.04
CN
BnOOC
N
Ph
CN
140.16
136.80
136.48
136.37
135.01
131.94
131.69
131.62
130.28
129.84
129.37
128.75
128.70
128.55
128.39
128.25
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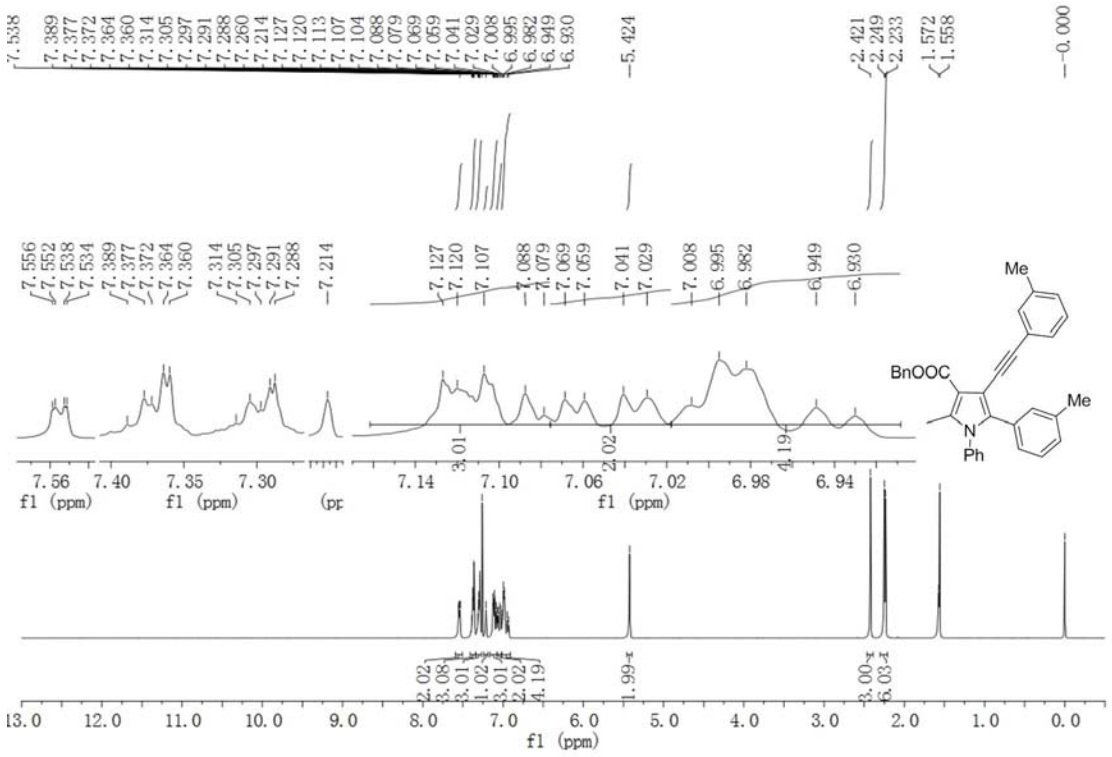
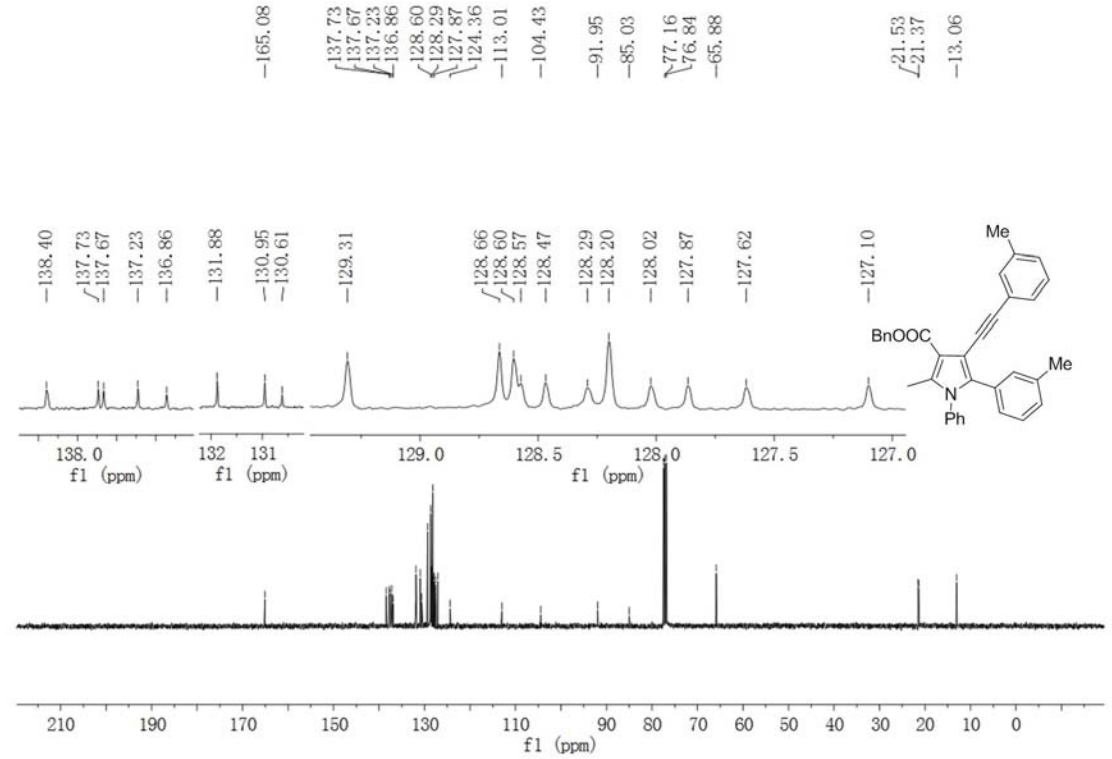
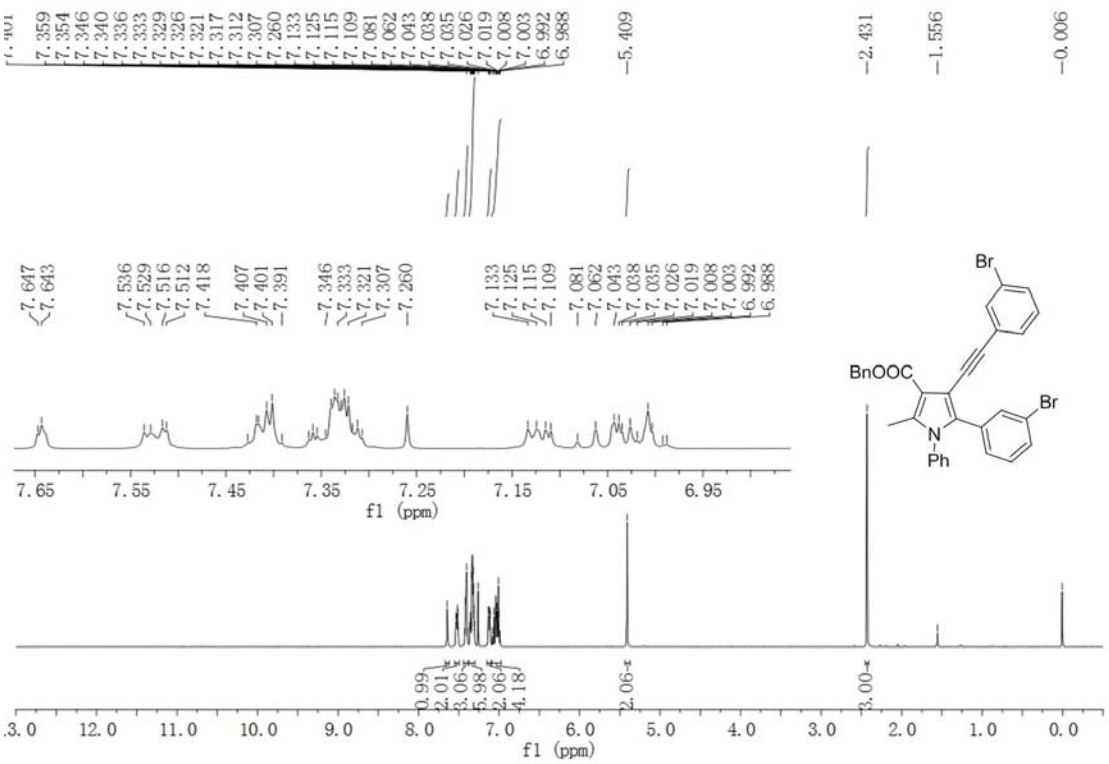
118.70
113.86
111.14
110.81
105.27
137
136
135
f1 (ppm)
131.5
130.5
129.5
128.5
f1 (ppm)
119
116
113
110
107
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Me
BnOOC
Me
N
Ph
f1 (ppm)


Me
BnOOC
Me
N
Ph
f1 (ppm)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7.333
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7.326
7.321
7.317
7.312
7.307
7.260
7.133
7.125
7.115
7.109
7.081
7.062
7.043
7.038
7.035
7.026
7.019
7.008
7.003
6.992
6.988
5.409
2.431
1.556
0.006
7.647
7.643
7.536
7.529
7.516
7.512
7.418
7.407
7.401
7.391
7.346
7.333
7.321
7.307
7.260
7.133
7.125
7.115
7.109
7.081
7.062
7.043
7.038
7.035
7.026
7.019
7.008
7.003
6.992
6.988
BnOOC
Br
Br
N
Ph
f1 (ppm)
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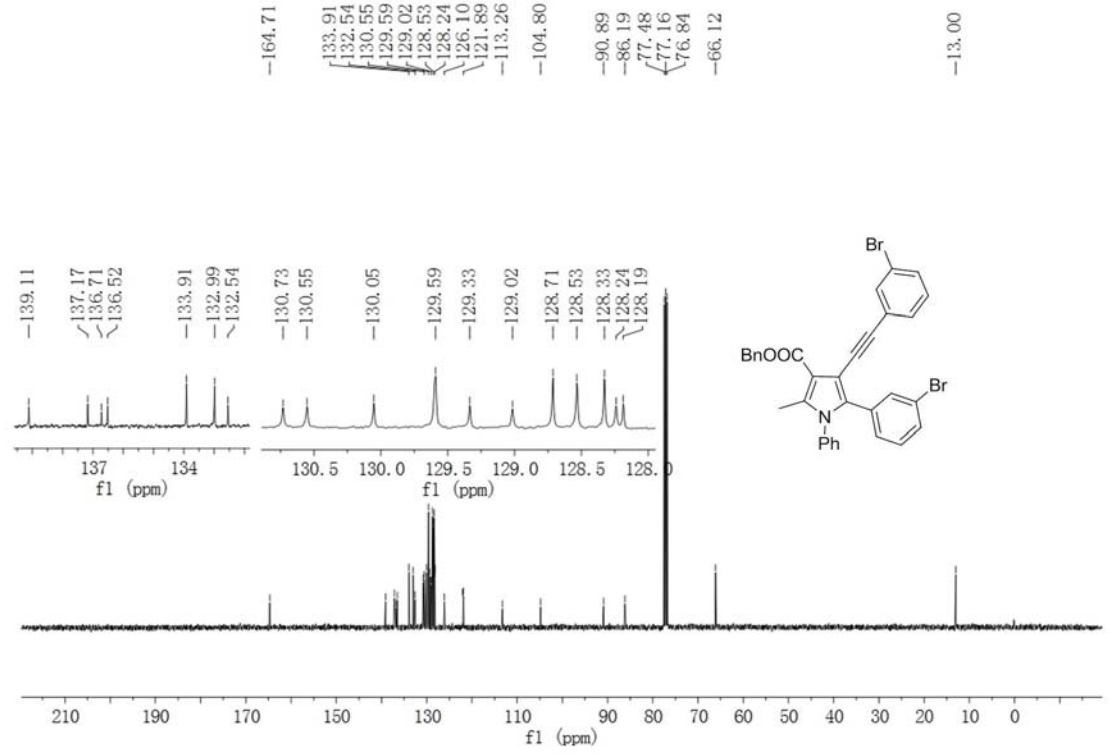
3.06
5.98
2.06
4.18
2.06
3.00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121.89
113.26
104.80
90.89
86.19
77.48
77.16
76.84
66.12
13.00
139.11
137.17
136.71
136.52
133.91
132.99
132.54
130.73
130.55
130.05
129.59
129.33
129.02
128.71
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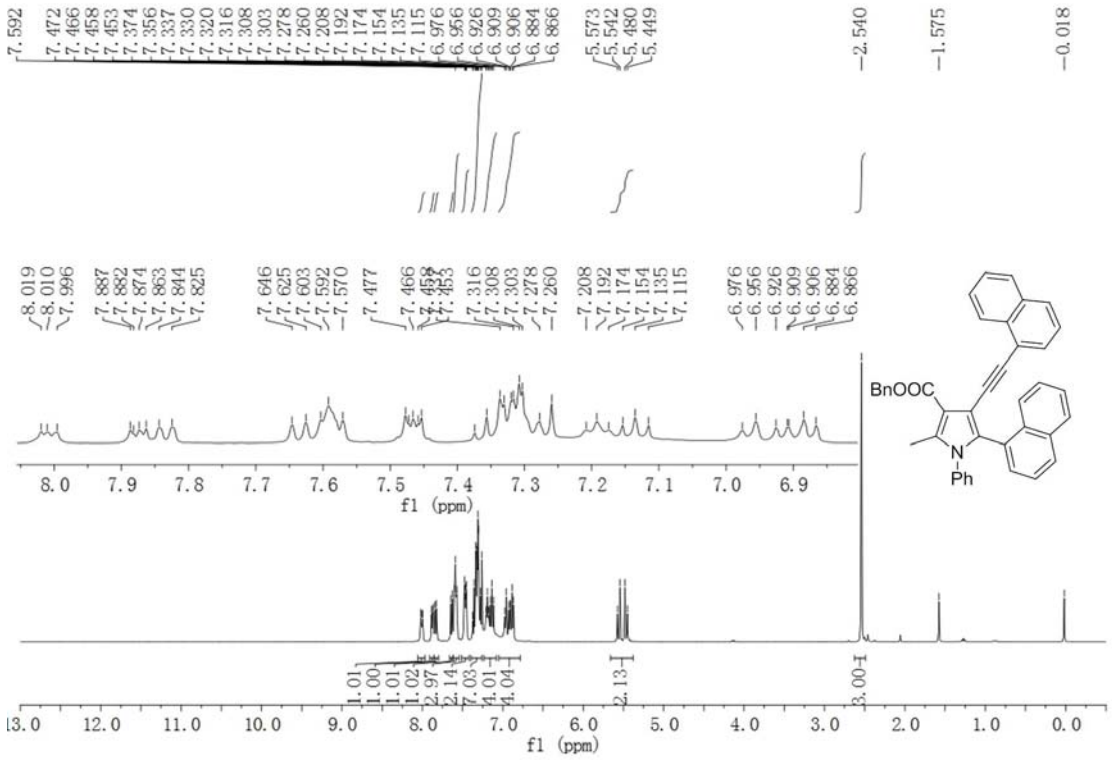
Br
N
Ph
f1 (ppm)
f1 (ppm)
f1 (ppm)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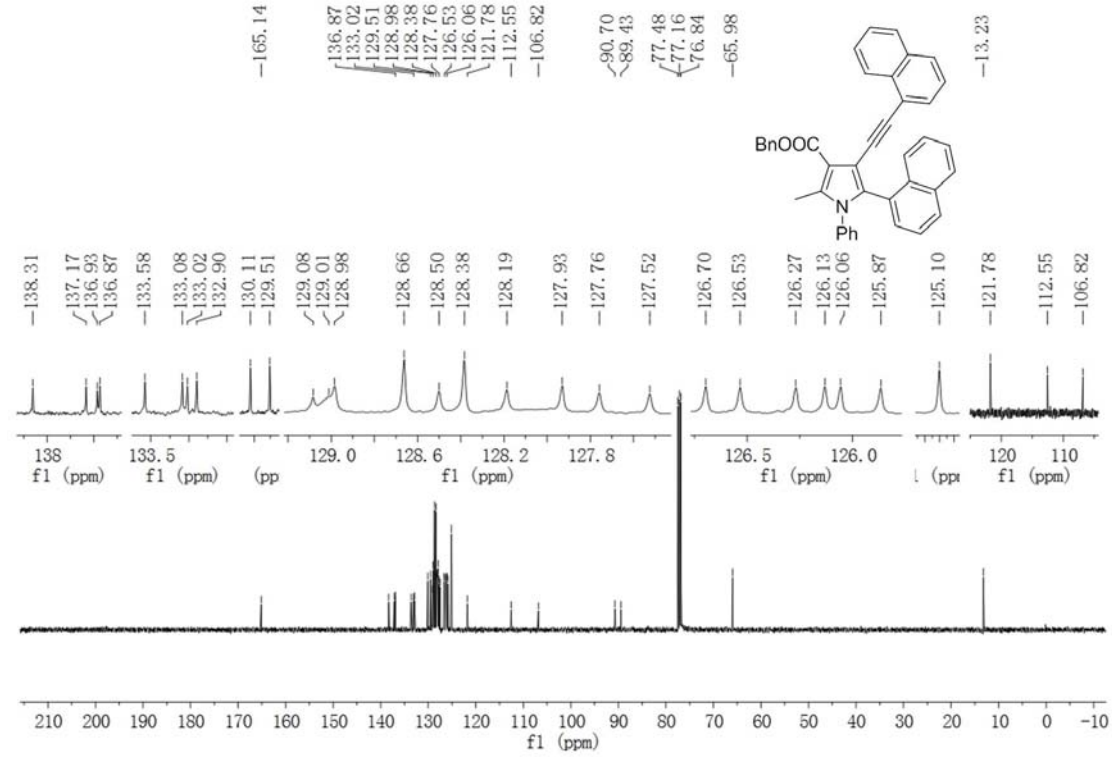
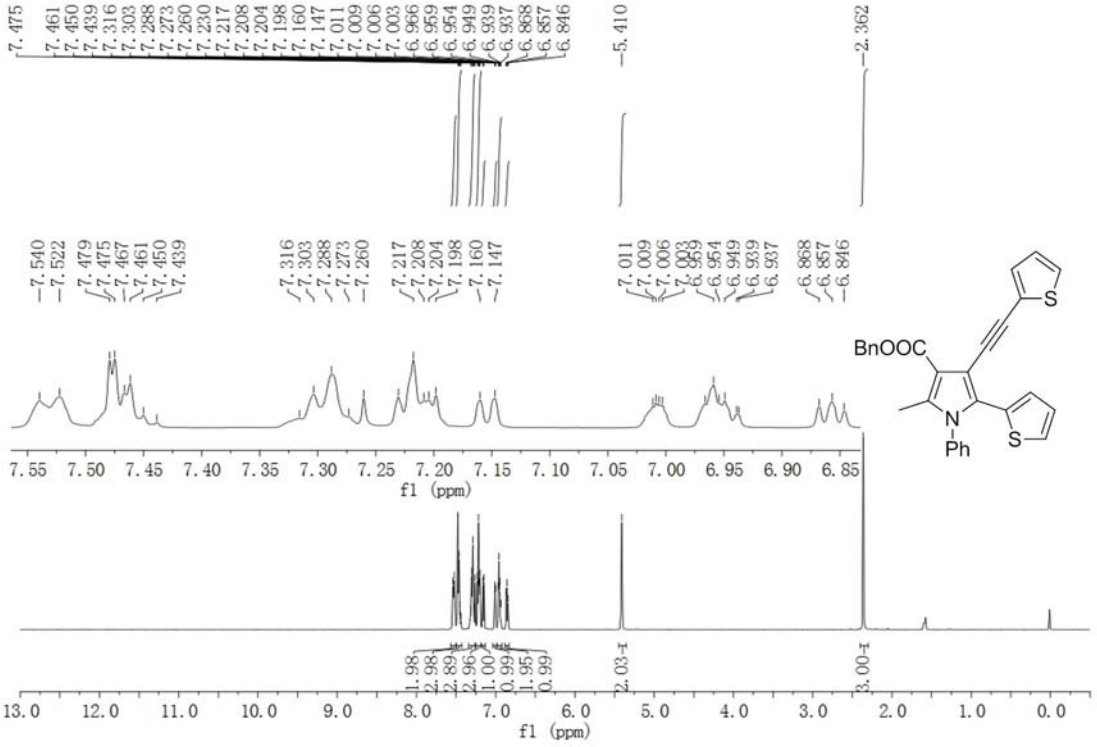
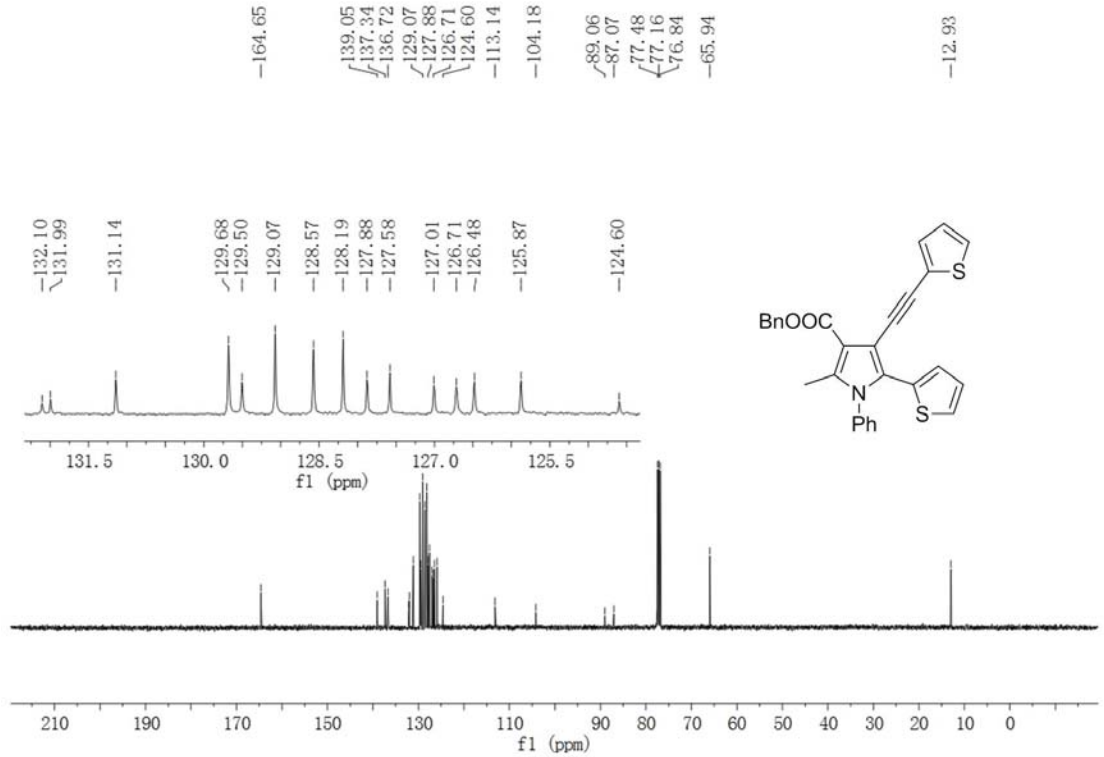
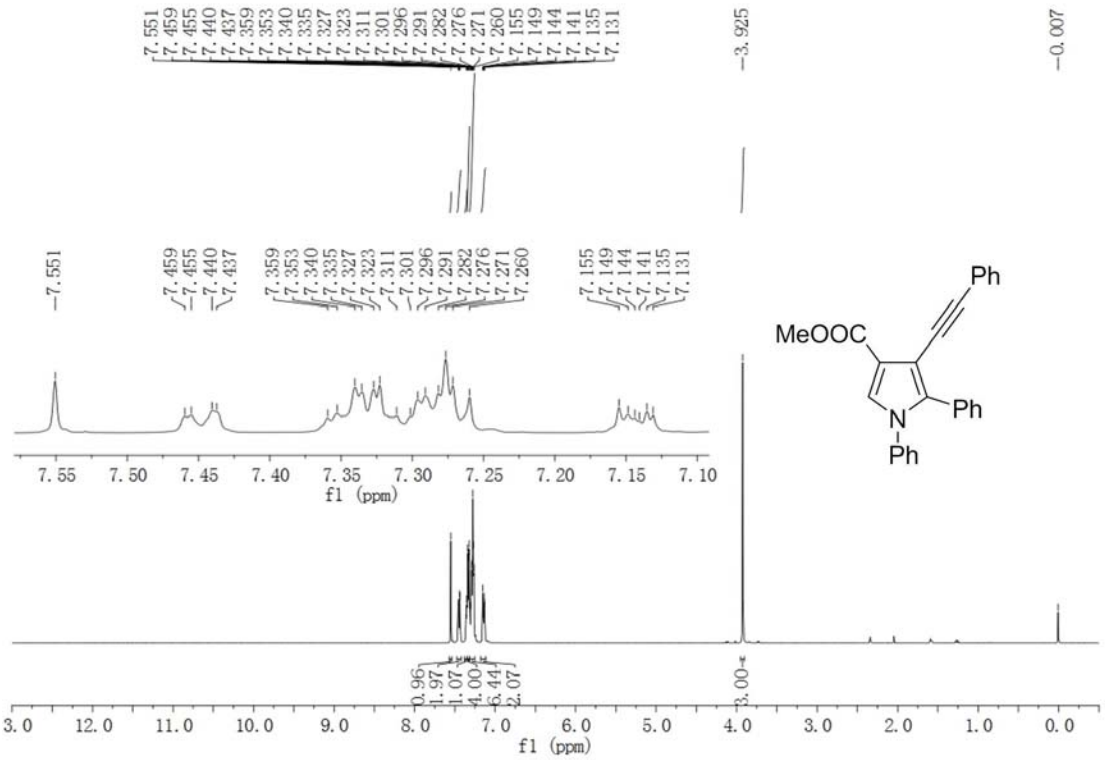
N
Ph
f1 (ppm)


BnOOC
N
Ph
f1 (ppm)


BnOOC
S
N
Ph
S
f1 (ppm)


BnOOC
S
N
Ph
S
f1 (ppm)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7.301
7.296
7.291
7.282
7.276
7.271
7.260
7.155
7.149
7.144
7.141
7.135
7.131
3.925
0.007
MeOOC
Ph
Ph
N
Ph
f1 (ppm)
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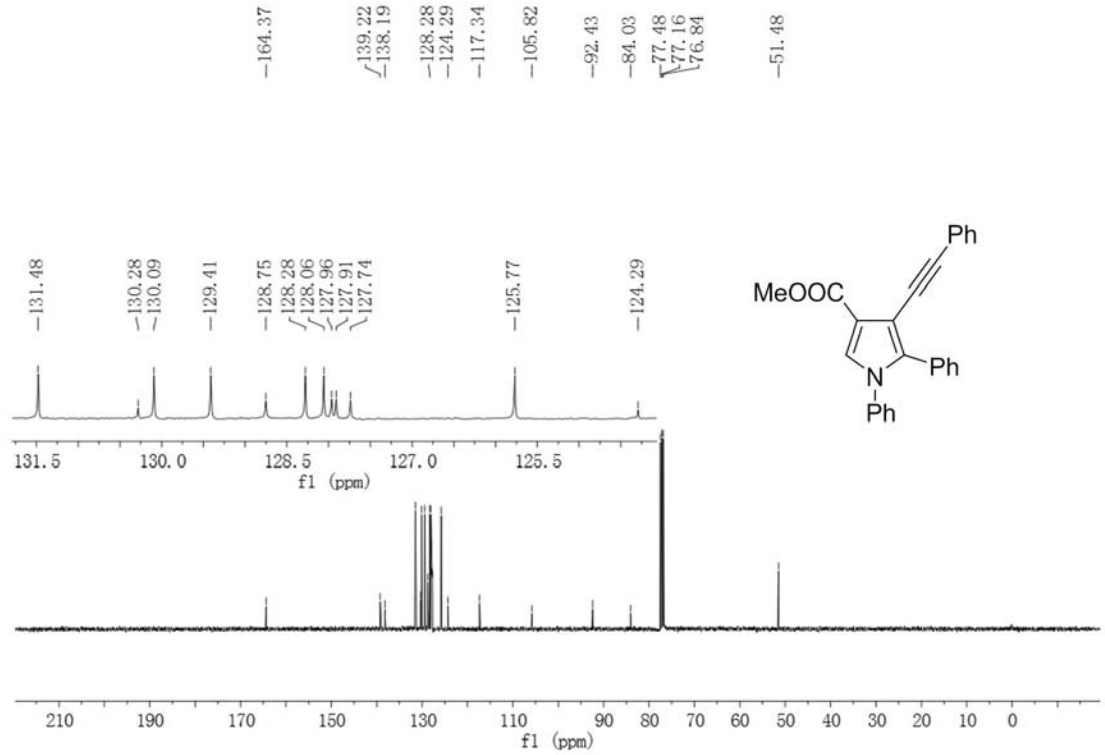
2.07
3.00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92.43
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77.48
77.16
76.84
51.48
131.48
130.28
130.09
129.41
128.75
128.28
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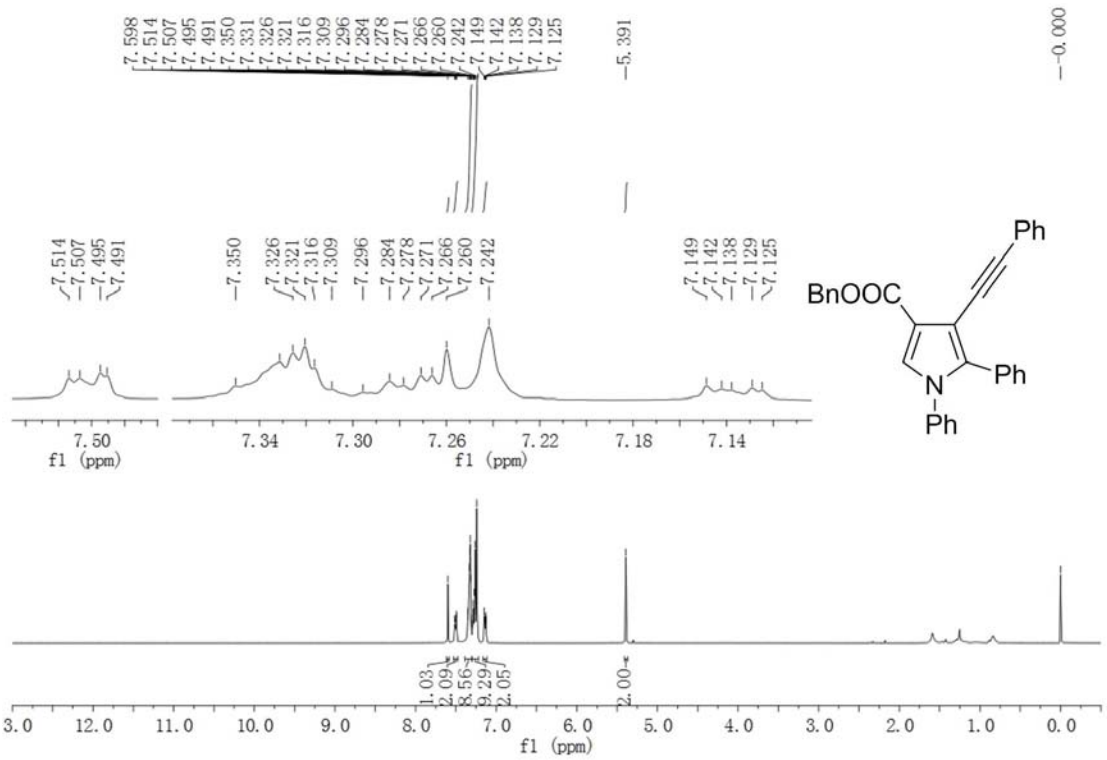
127.91
127.74
125.77
124.29
MeOOC
Ph
Ph
N
Ph
f1 (ppm)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7.296
7.284
7.278
7.271
7.266
7.260
7.242
7.149
7.142
7.138
7.129
7.125
5.391
0.000
BnOOC
Ph
Ph
N
Ph
f1 (ppm)
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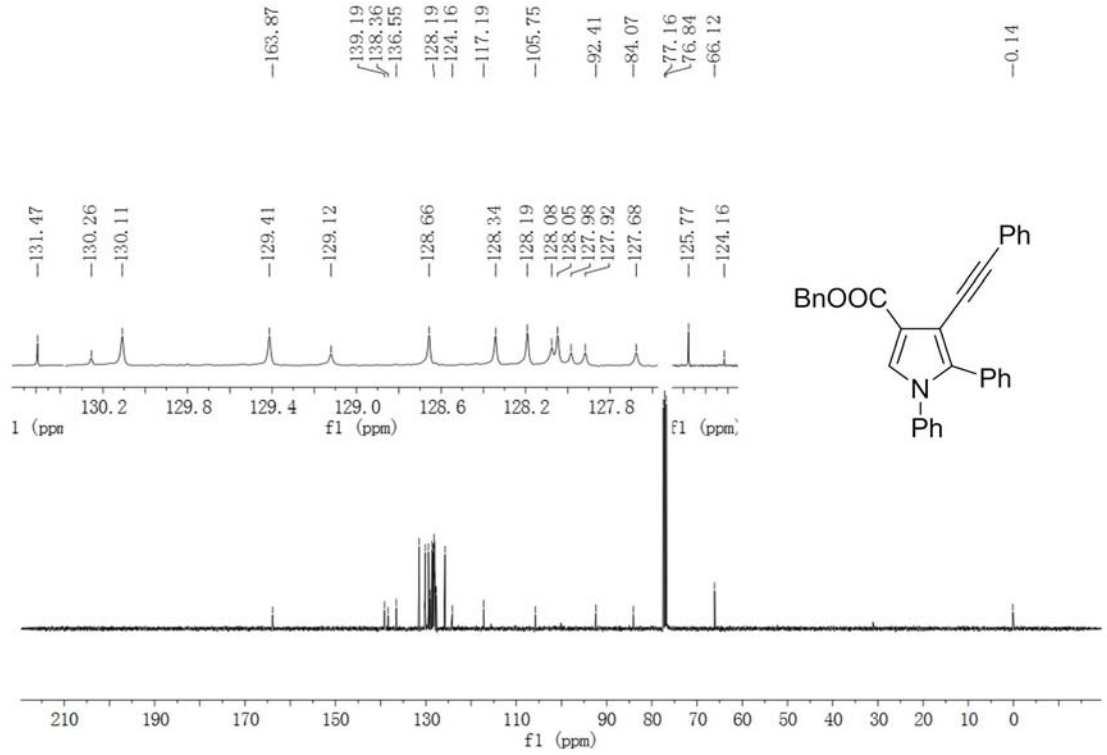
2.09
8.56
9.29
2.05
2.00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84.07
77.16
76.84
66.12
0.14
131.47
130.26
130.11
129.41
129.12
128.66
128.34
128.19
128.08
128.05
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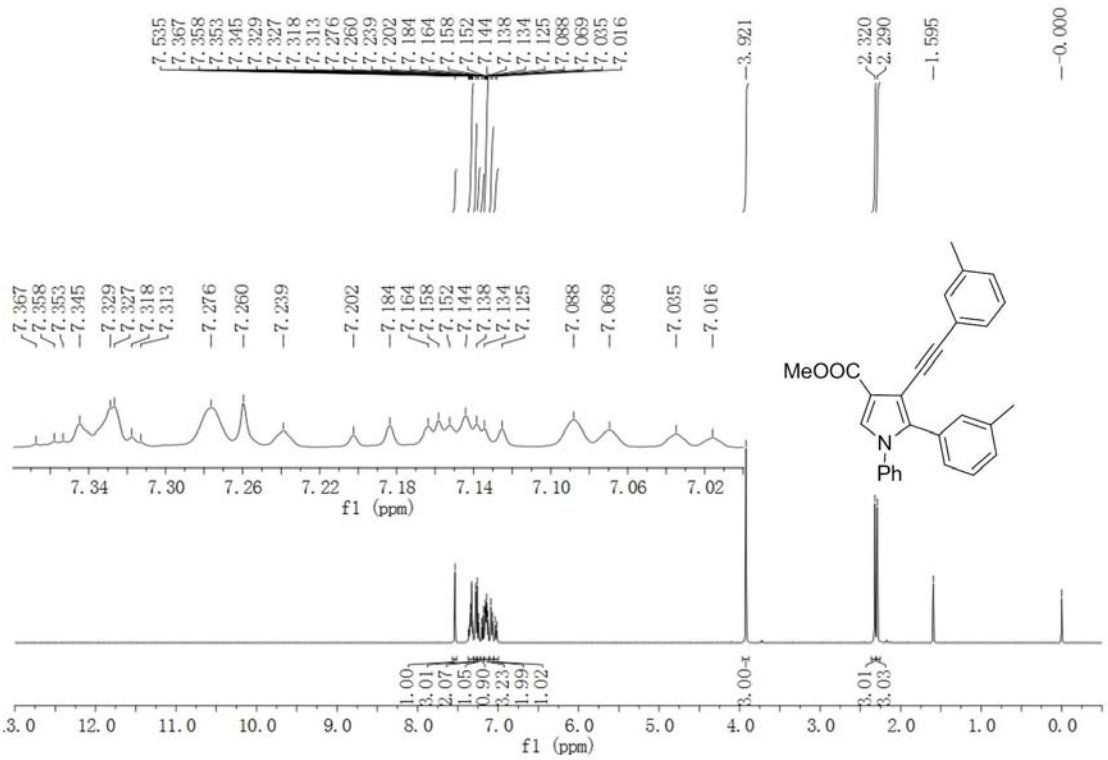
127.92
127.68
125.77
124.16
BnOOC
Ph
Ph
N
Ph
f1 (ppm)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7.329
7.327
7.318
7.313
7.276
7.260
7.239
7.202
7.184
7.164
7.158
7.152
7.144
7.138
7.134
7.125
7.088
7.069
7.035
7.016
3.921
2.320
2.290
1.595
0.000
MeOOC
N
Ph
f1 (ppm)
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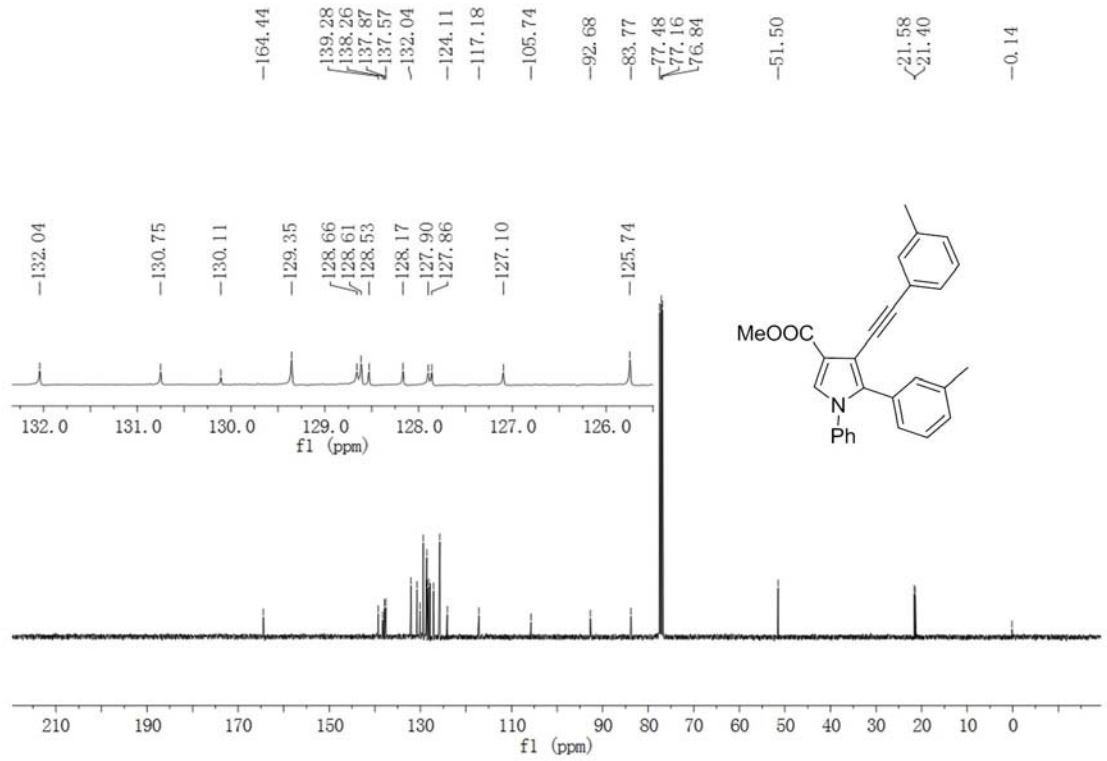
2.07
1.05
0.90
3.23
1.99
1.02
3.00
3.01
3.03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137.87
137.57
132.04
124.11
117.18
105.74
92.68
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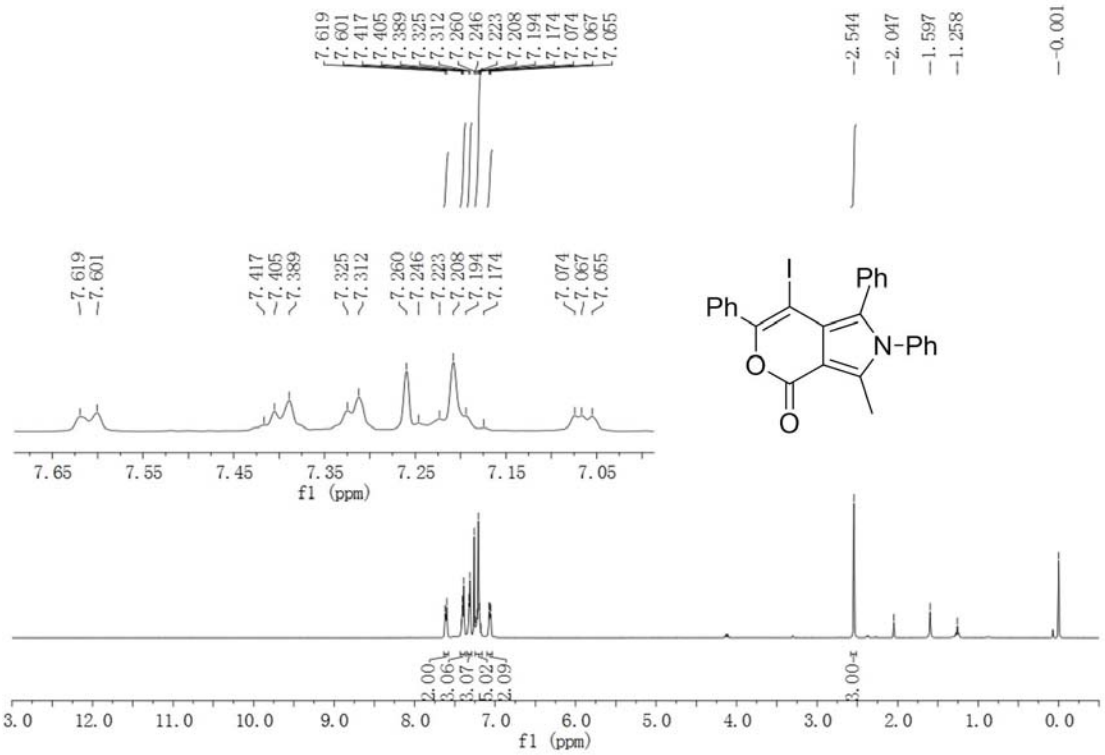
77.16
76.84
51.50
21.58
21.40
0.14
MeOOC
N
Ph
f1 (ppm)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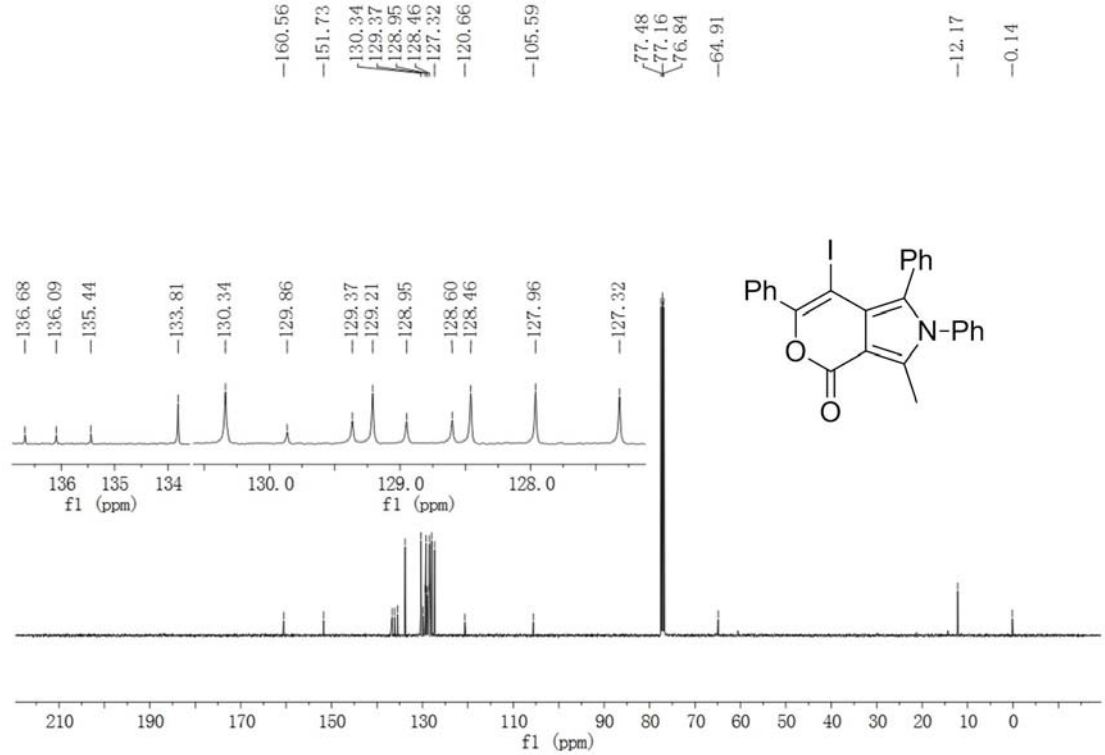
7.389
7.325
7.312
7.260
7.246
7.223
7.208
7.194
7.174
7.074
7.067
7.055
2.544
2.047
1.597
1.258
0.001
Ph
Ph
N-Ph
O
O
f1 (ppm)
2.00
3.06
3.07
5.02
2.09
3.00
f1 (ppm)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12.17
0.14
136.68
136.09
135.44
133.81
130.34
129.86
129.37
129.21
128.95
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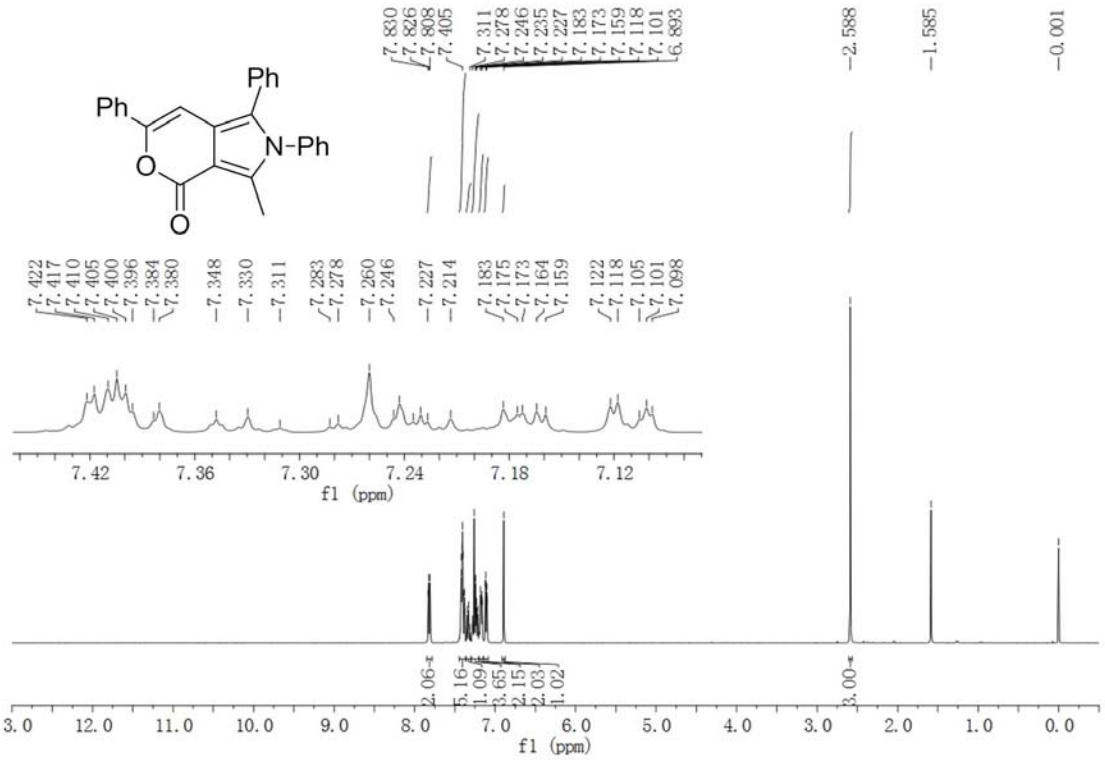
Ph
Ph
N-Ph
O
O
f1 (ppm)
f1 (ppm)
f1 (ppm)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N-Ph
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7.183
7.173
7.159
7.118
7.101
6.893
2.588
1.585
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7.405
7.400
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7.380
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7.278
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7.227
7.214
7.183
7.175
7.173
7.164
7.159
7.122
7.118
7.105
7.101
7.098
7.42
7.36
7.30
7.24
7.18
7.12
f1 (ppm)
2.06
5.16
1.09
3.65
2.15
2.03
1.02
3.00
3.0
12.0
11.0
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1.0
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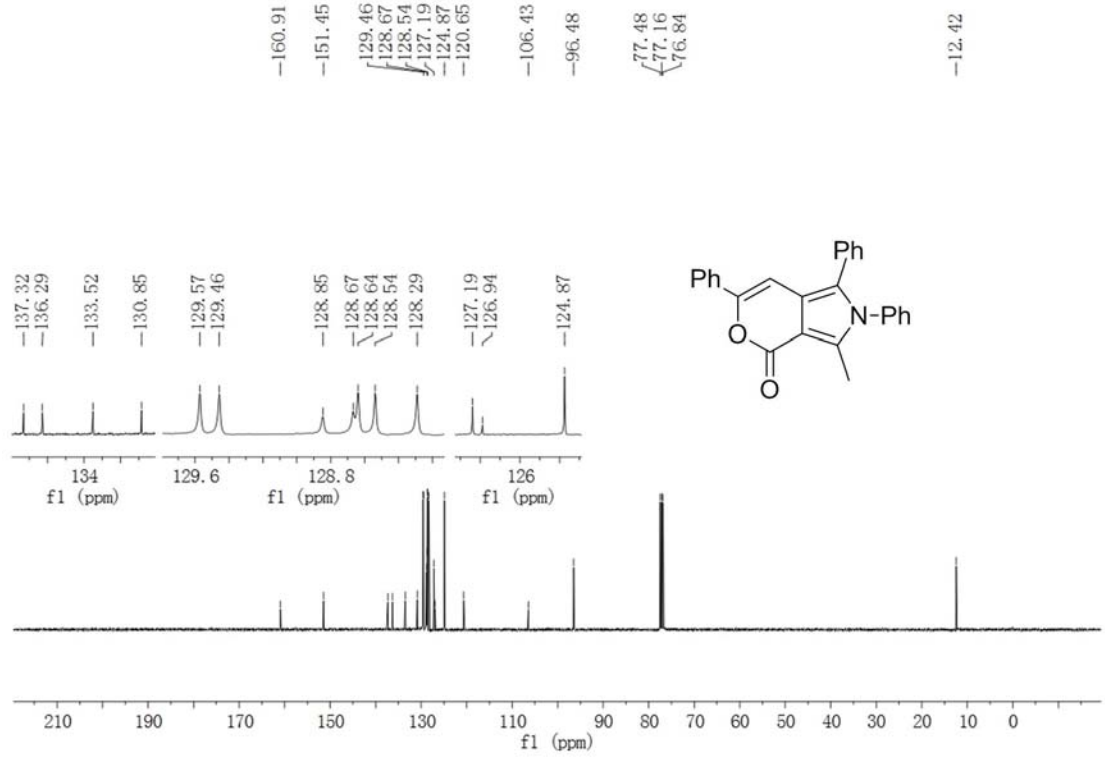
f1 (ppm)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128.54
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120.65
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96.48
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77.16
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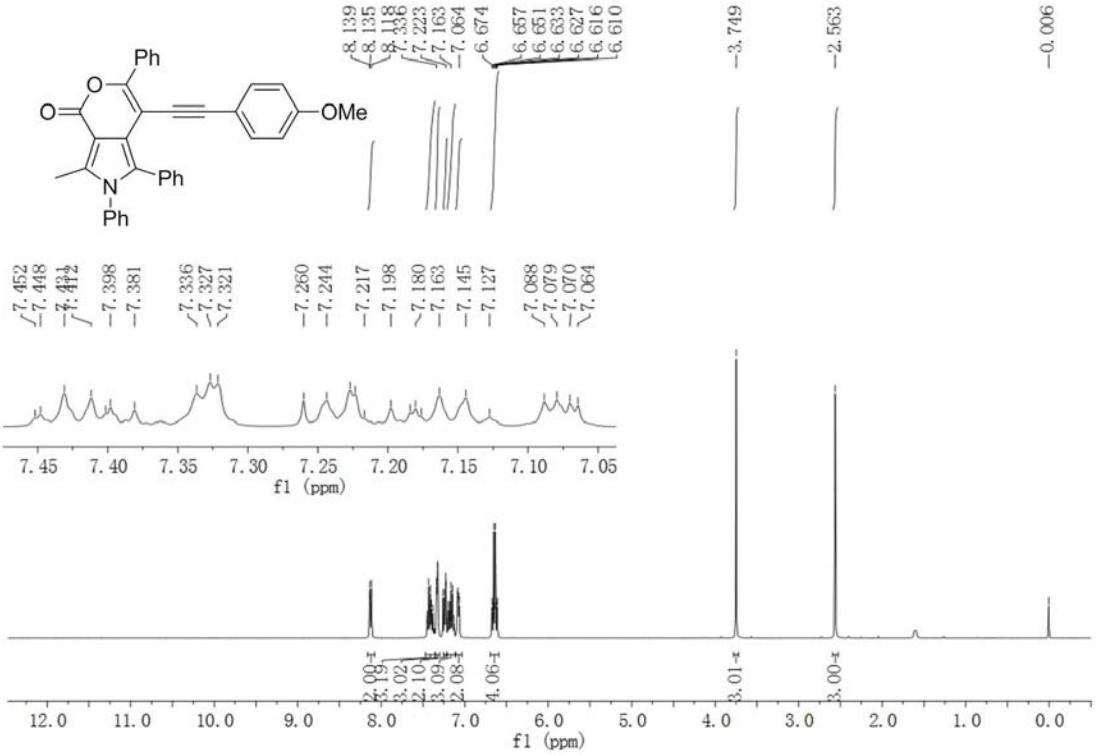
12.42
137.32
136.29
133.52
130.85
129.57
129.46
128.85
128.67
128.64
128.54
128.29
127.19
126.94
124.87
Ph
Ph
N-Ph
O
O
134
f1 (ppm)
129.6
128.8
f1 (ppm)
126
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Ph
O
O
OMe
Ph
N
Ph
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8.118
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7.223
7.163
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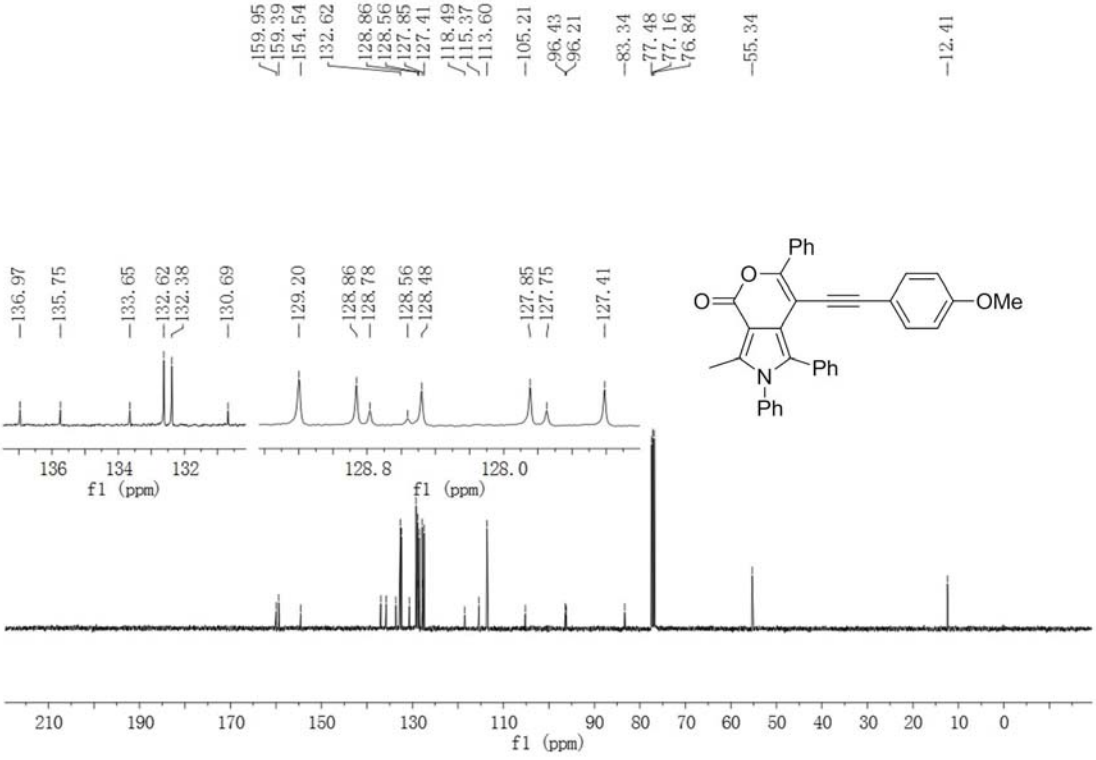
6.674
6.657
6.651
6.633
6.627
6.616
6.610
3.749
2.563
0.006
7.452
7.448
7.398
7.381
7.336
7.327
7.321
7.260
7.244
7.217
7.198
7.180
7.163
7.145
7.127
7.088
7.079
7.070
7.064
7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05
f1 (ppm)
2.00
2.15
3.02
2.10
3.09
2.08
4.06
3.01
3.00
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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127.41
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115.37
113.60
105.21
96.43
96.21
83.34
77.48
77.16
76.84
55.34
12.41
136.97
135.75
133.65
132.62
132.38
130.69
129.20
128.86
128.78
128.56
128.48
127.85
127.75
127.41
Ph
O
O
OMe
Ph
N
Ph
136 134 132
f1 (ppm)
128.8 128.0
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)