Elemental Sulfur-Incorporated Cyclizations of Pyrrolidines Leading to Thienopyrroles

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Contents

1. Optimization of the reaction conditions……S2

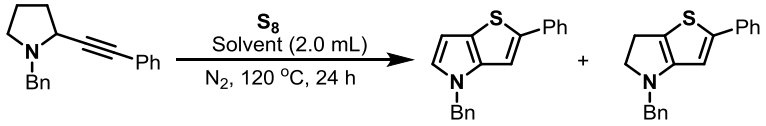
2. EPR experiment procedure.……...S3

3. ^{1}H NMR and ^{13}C {^{1}H} NMR copies of substrates…… …...S4

4. ^{1}H NMR and ^{13}C {^{1}H} NMR copies of products……...S45

5. Single-Crystal X-ray diffraction……...….S91

Table S1. Optimization of the reaction conditions.[a]



1a **2a** **2a'**

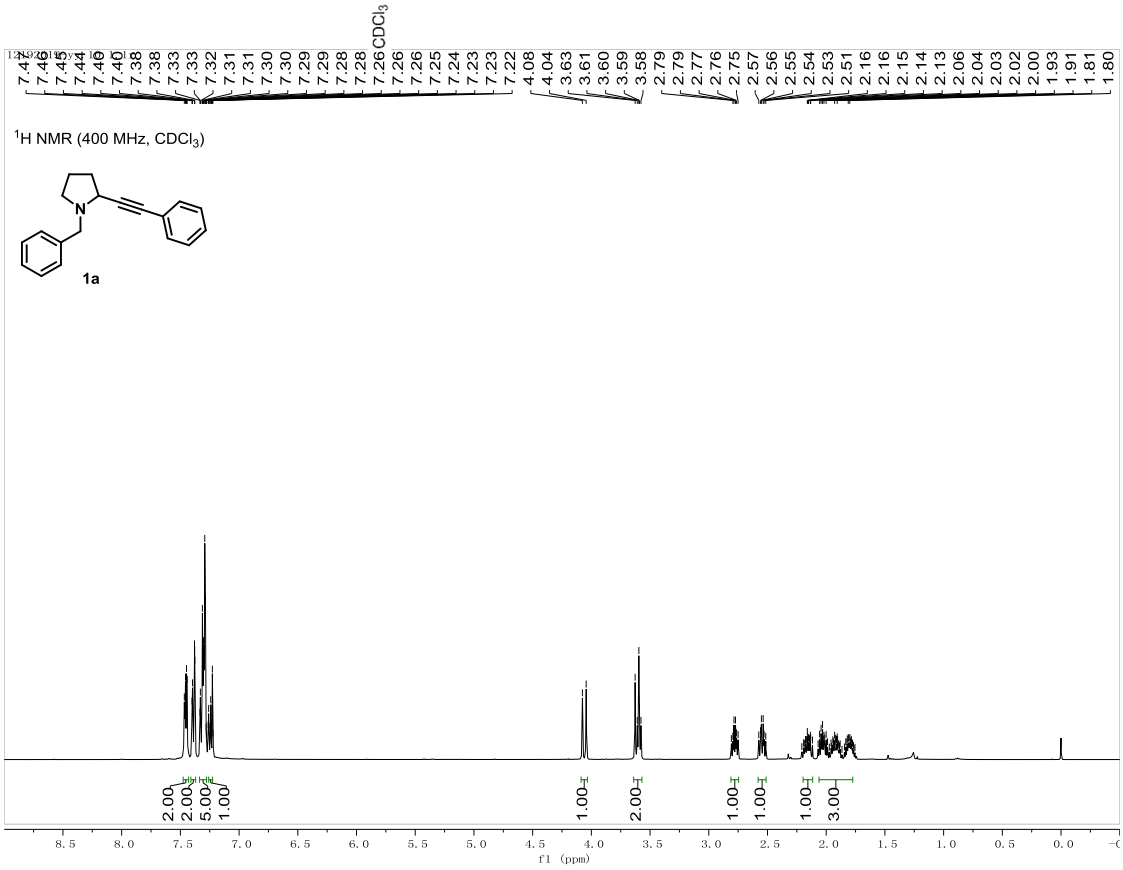
Entry	S_8 (equiv)	Base (equiv)	Solvent	t (h)	T (°C)	Yield (%) **2a'**	Yield (%) **2a**
1	S_8 (1.0)	K_2CO_3 (2.0)	1,4-dioxane	24	100	27	0
2	S_8 (1.5)	K_2CO_3 (2.0)	1,4-dioxane	24	100	41	8
3	S_8 (1.0)	NaO^{t}Bu (2.0)	1,4-dioxane	24	100	15	7
4	S_8 (1.0)	K_2CO_3 (2.0)	1,4-dioxane	36	100	22	4
5	S_8 (1.0)	K_2CO_3 (2.0)	1,4-dioxane	48	100	32	13
6	S_8 (1.5)	K_2CO_3 (2.0)	1,4-dioxane	36	100	30	15
7	S_8 (1.5)	K_2CO_3 (1.0)	1,4-dioxane	24	100	29	18
8	S_8 (1.5)		1,4-dioxane	24	100	39	17
9	S_8 (1.5)		1,4-dioxane	24	110	37	30
10	**S_8 (1.5)**		**1,4-dioxane**	**24**	**120**	0	**74**
11	S_8 (1.5)		1,4-dioxane	36	100	0	64
13	S_8 (1.5)		1,4-dioxane	36	110	0	64
14	S_8 (1.5)		1,4-dioxane	36	120	0	63
15	S_8 (1.0)		1,4-dioxane	24	120	0	43
16	S_8 (0.50)		1,4-dioxane	24	120	0	41
17	S_8 (1.5)		THF	24	120	19	55
18	S_8 (1.5)		Toluene	24	120	0	37
19	S_8 (1.5)		DMF	24	120	0	53
20	S_8 (1.5)		DME	24	120	0	71

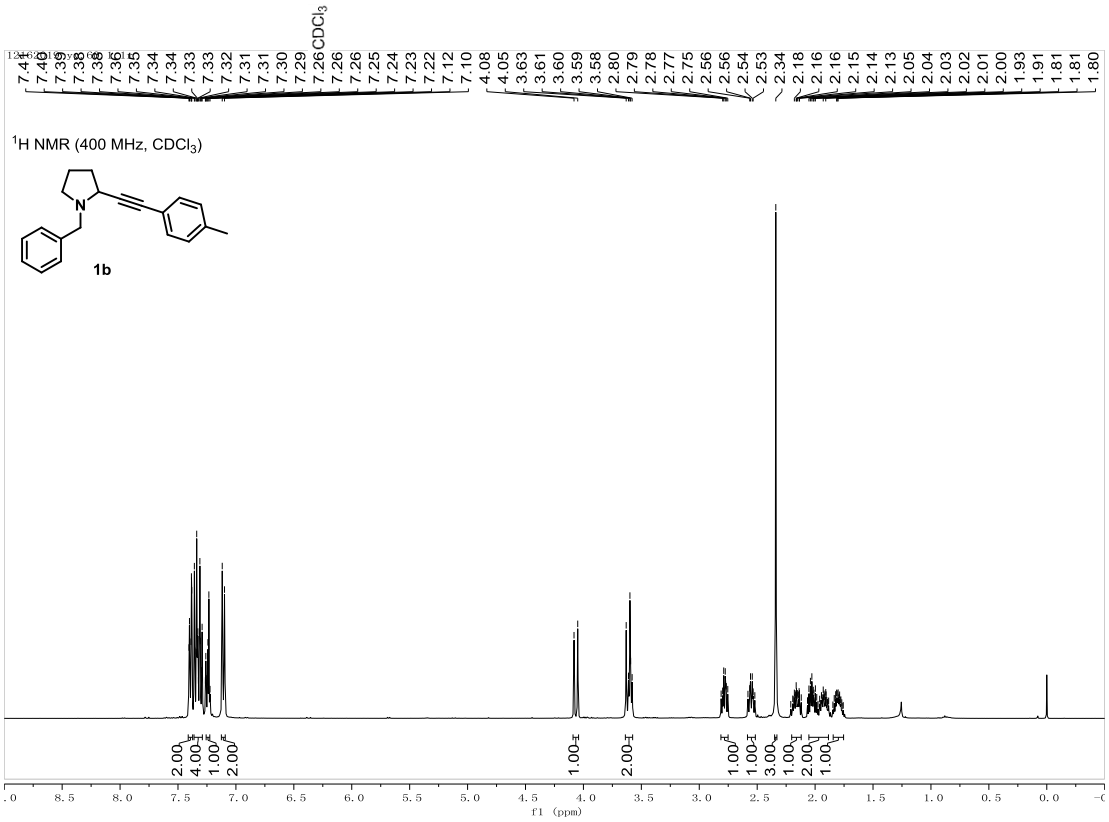
[a] Standard condition: **1a** (0.30 mmol), **S_8** (1.5 equiv), solvent (2.0 mL), N_2, 120 °C, 24 h.

2. EPR experiment procedure for interaction of 4-benzyl-2-phenyl-5, 6-dihydro-4*H*-thieno[3,2-*b*]pyrrole (1a) with elemental sulfur.

1-benzyl-2-(phenylethynyl)pyrrolidine (78.4 mg, 0.30 mmol) and elemental sulfur $\mathbf{S_8}$ (115.2 mg, 0.45 mmol) were combined in a 50 mL flame-dried Young-type tube equipped with a stir bar, and then the tube was sealed. Next, the Schlenk tube was purged three times with N_2. Then, 1,4-dioxane (2.0 mL) was injected into the Schlenk tube with a syringe under N_2 atmosphere. The contents of the Schlenk tube were then allowed to stir at 120 ℃ by using a heating mantle for 1.0 h. Then, DMPO was added to the mixture and preserved in liquid nitrogen for EPR examination. No organic radical was observed.

3. ^{1}H NMR and ^{13}C {^{1}H} NMR copies of substrates

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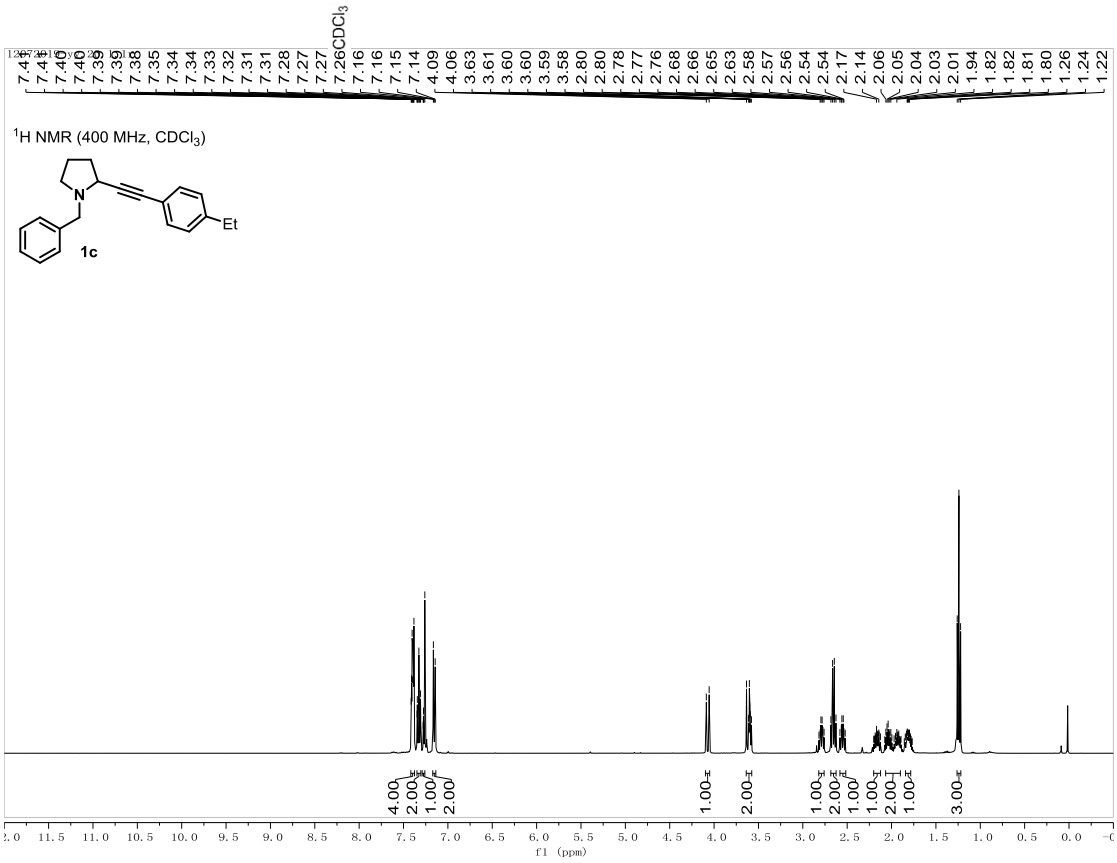
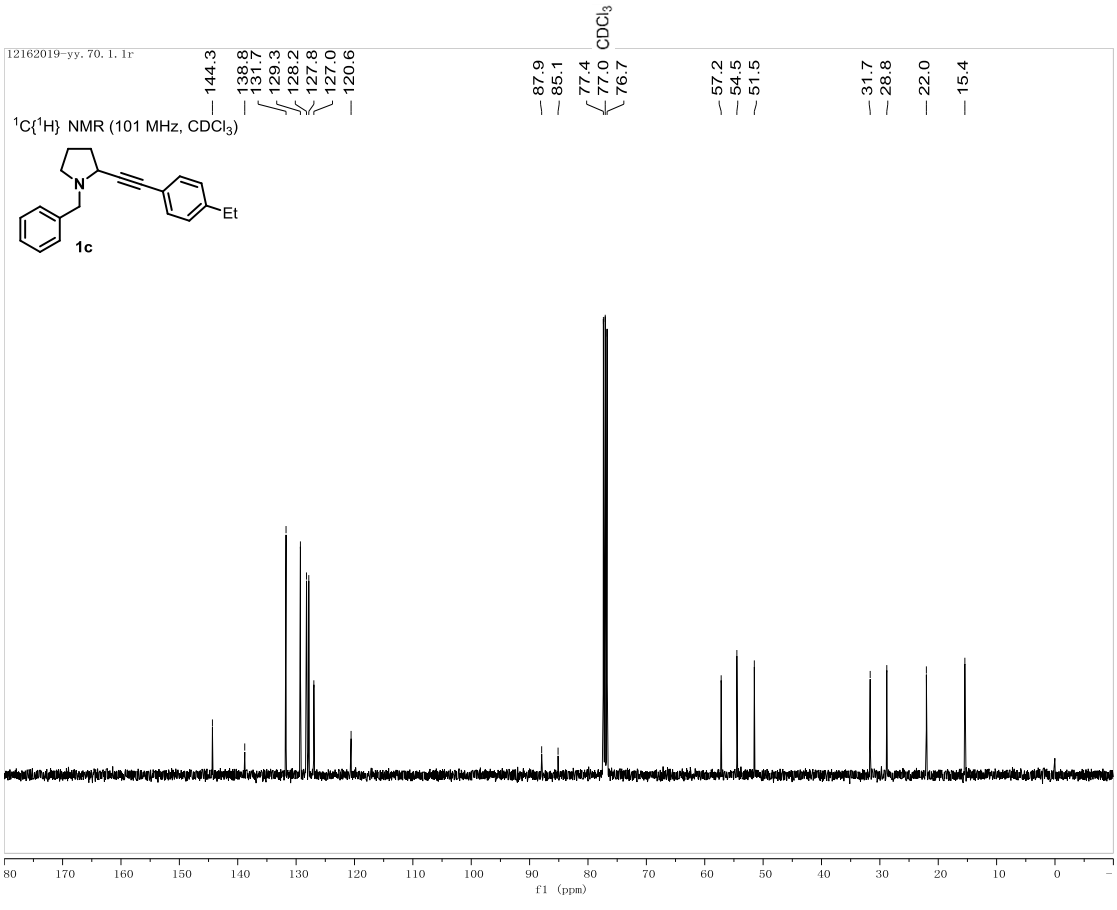
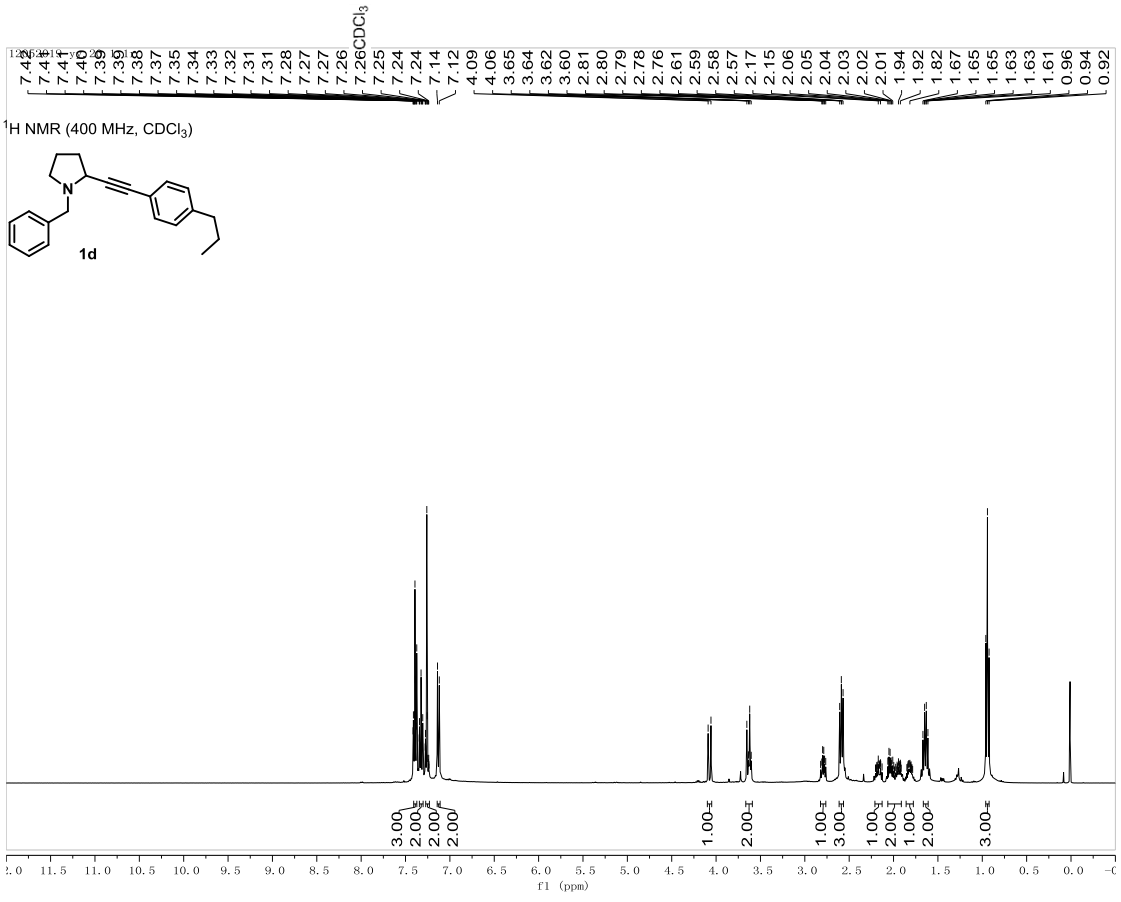
1b
$CDCl_3$
f1 (ppm)



^{1}H NMR (400 MHz, CDCl$_3$)
1c
Et
CDCl$_3$
f1 (ppm)



^{1}C{^{1}H} NMR (101 MHz, CDCl$_3$)
1c
Et
CDCl$_3$
f1 (ppm)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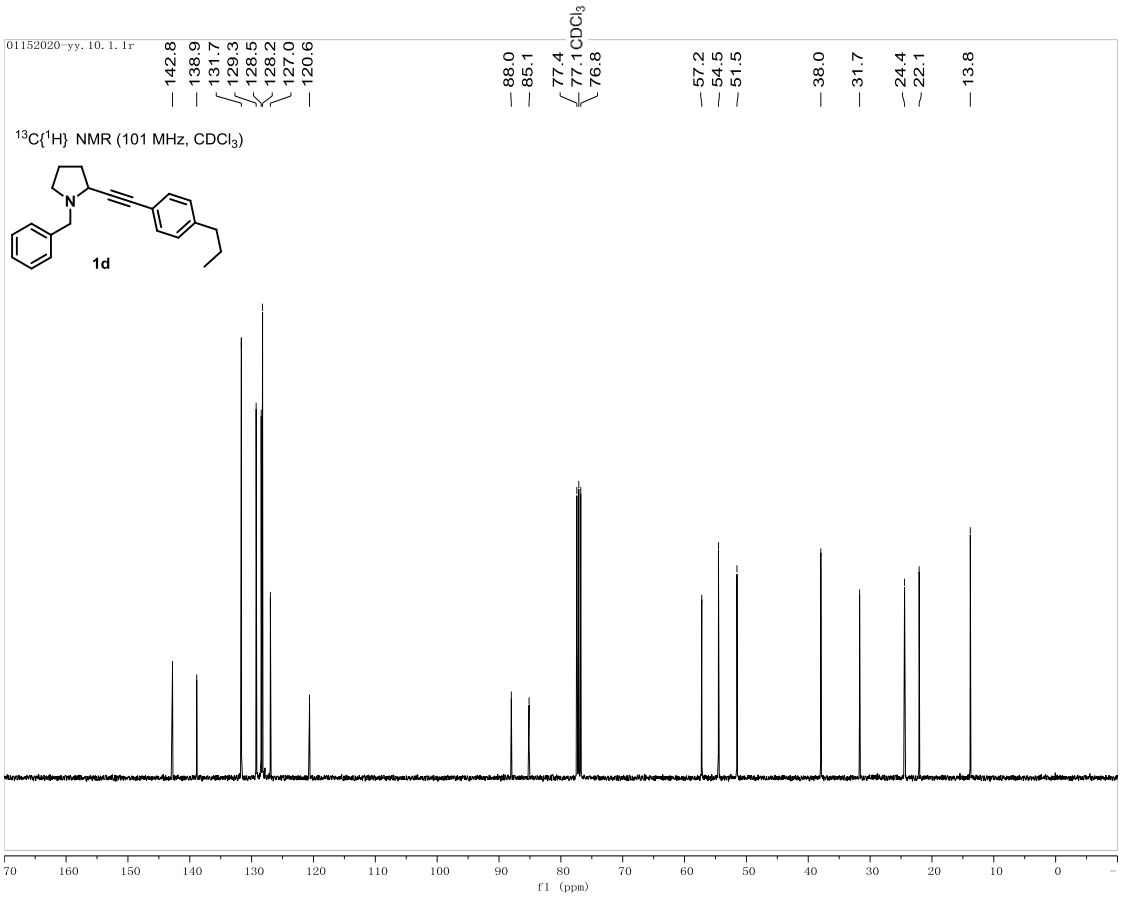
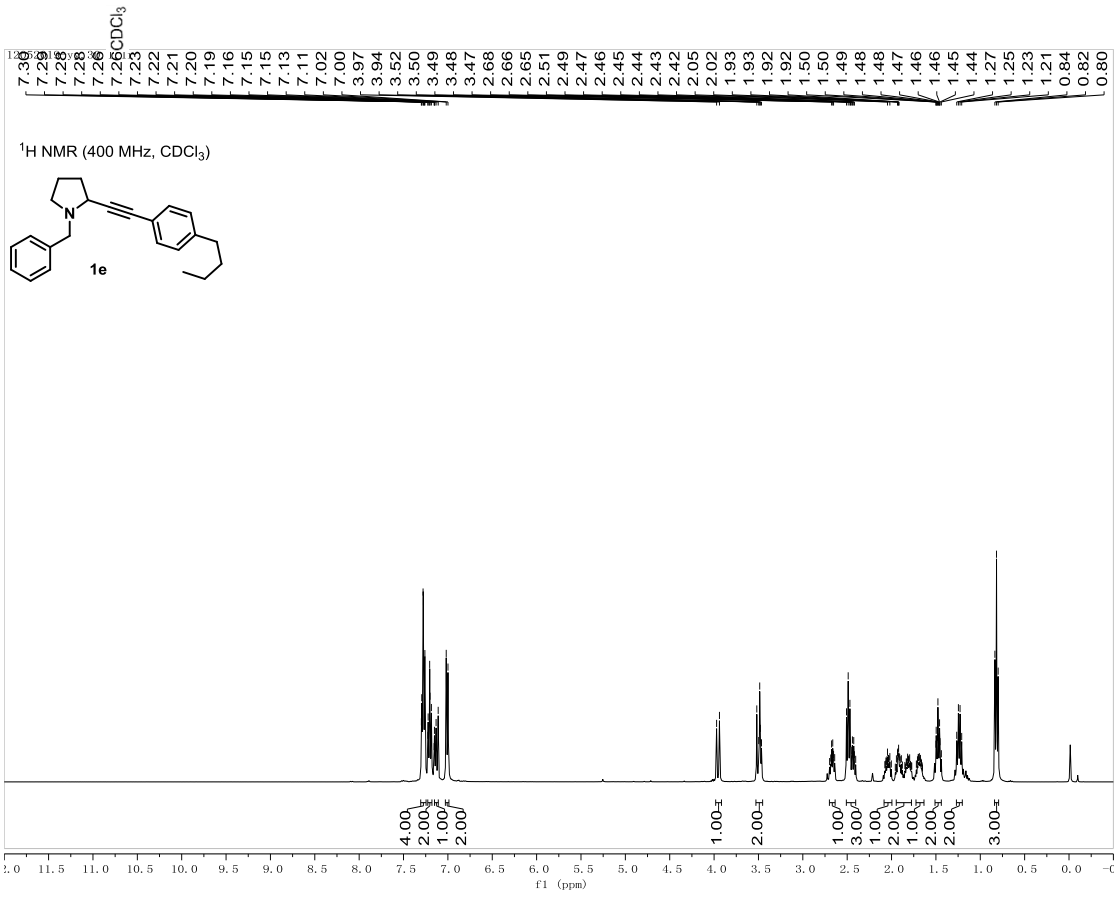
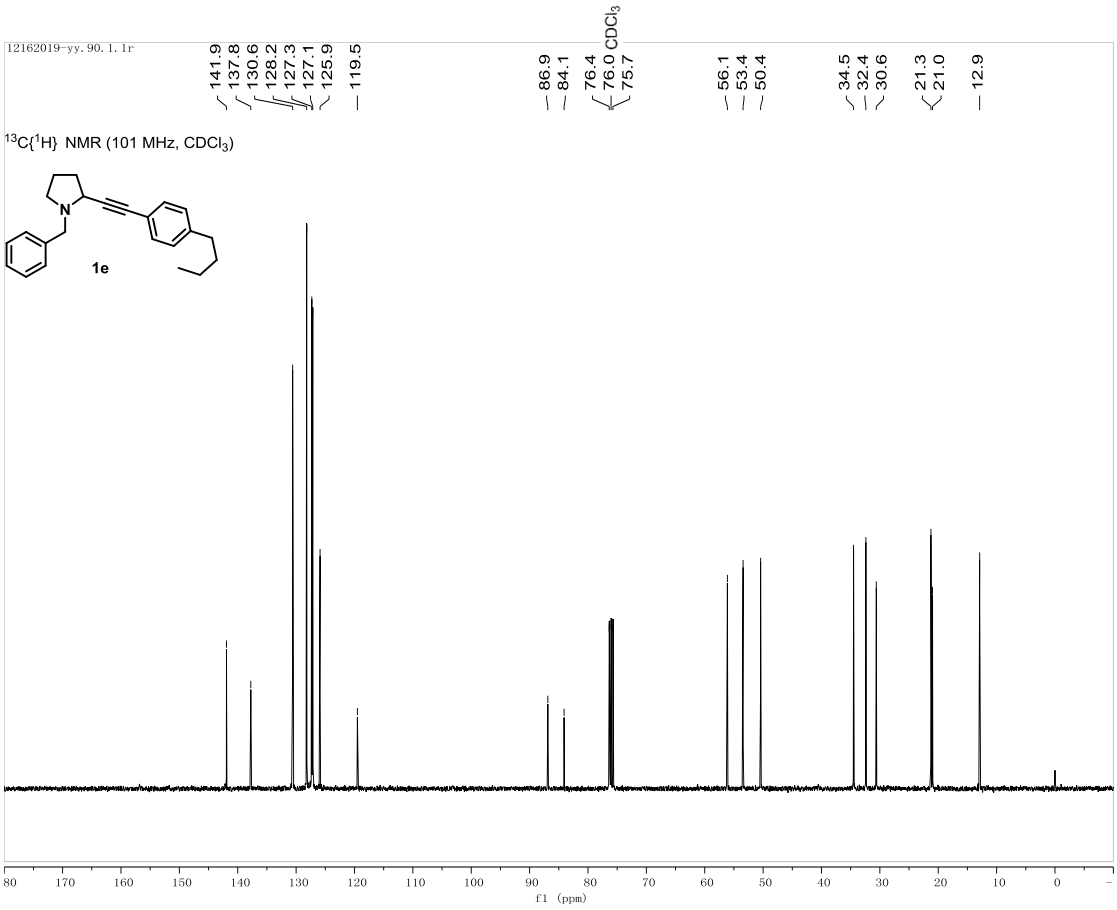
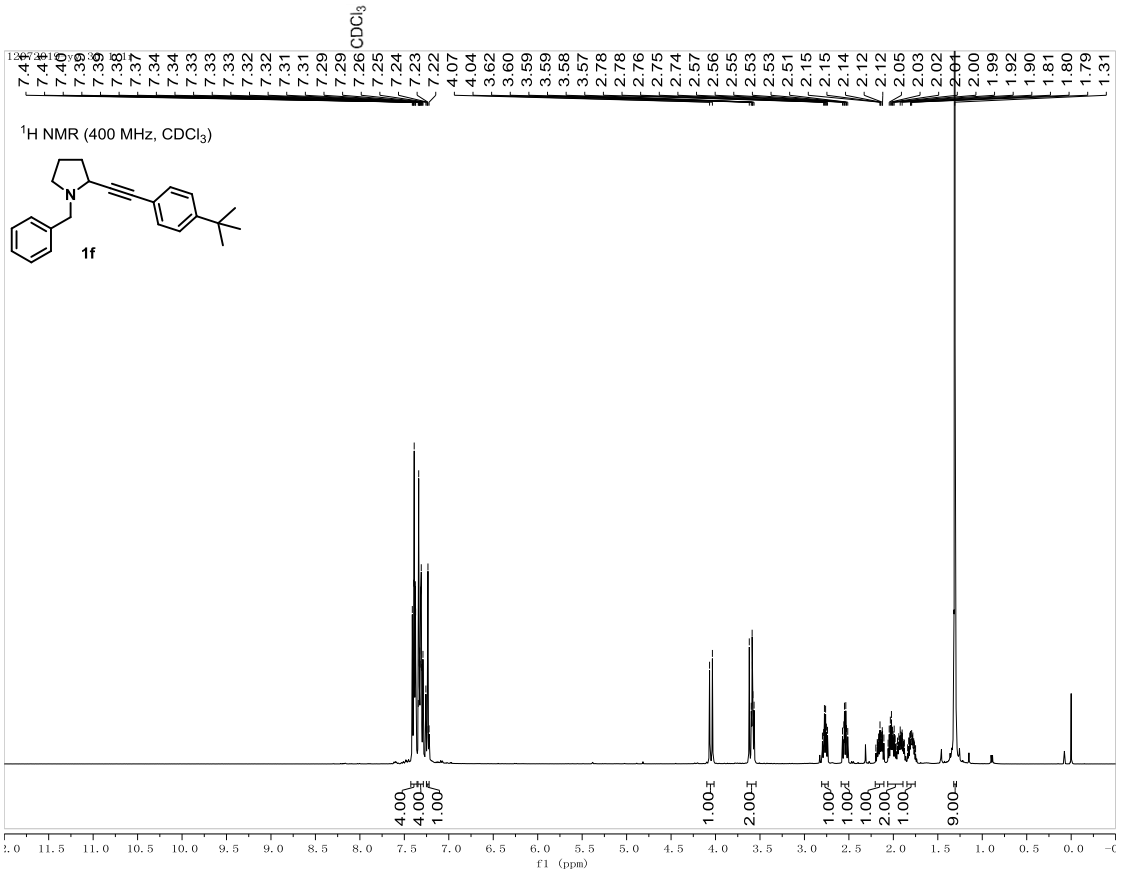
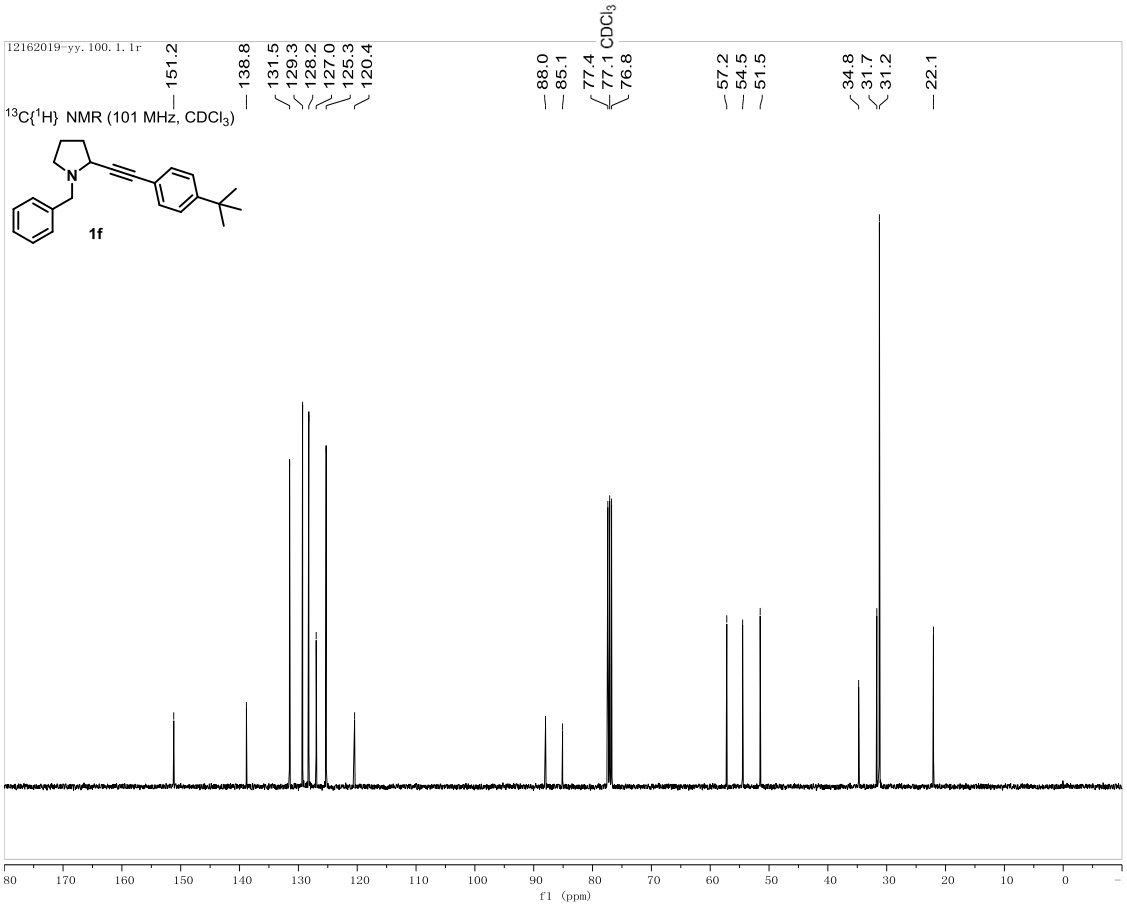
1H NMR (400 MHz, CDCl3)
1d
3.00 2.00 2.00 2.00 1.00 2.00 1.00 3.00 1.00 2.00 1.00 2.00 3.00
f1 (ppm)

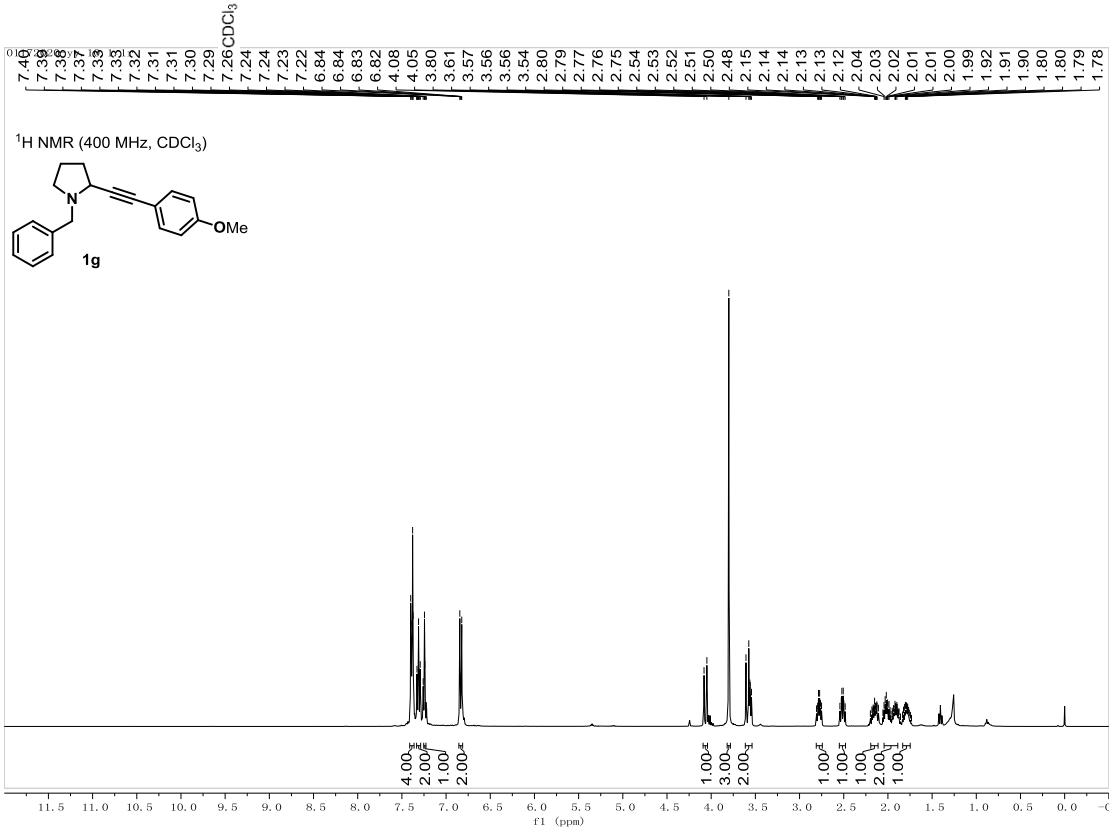

01152020-yy. 10. 1. 1r
142.8 138.9 131.7 129.3 128.5 128.2 127.0 120.6 88.0 85.1 77.4 77.1 CDCl3 76.8 57.2 54.5 51.5 38.0 31.7 24.4 22.1 13.8
13C{1H} NMR (101 MHz, CDCl3)
1d
f1 (ppm)

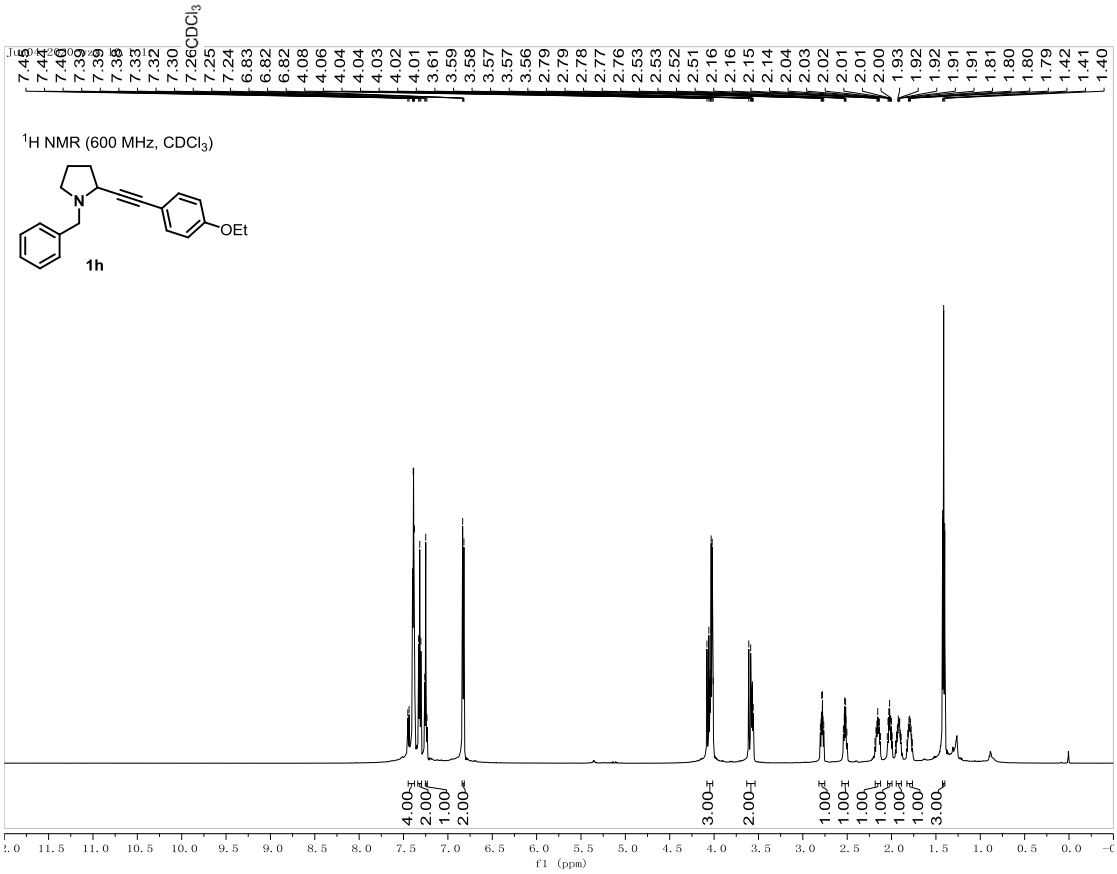

^{1}H NMR (400 MHz, $CDCl_3$)
1e
f1 (ppm)

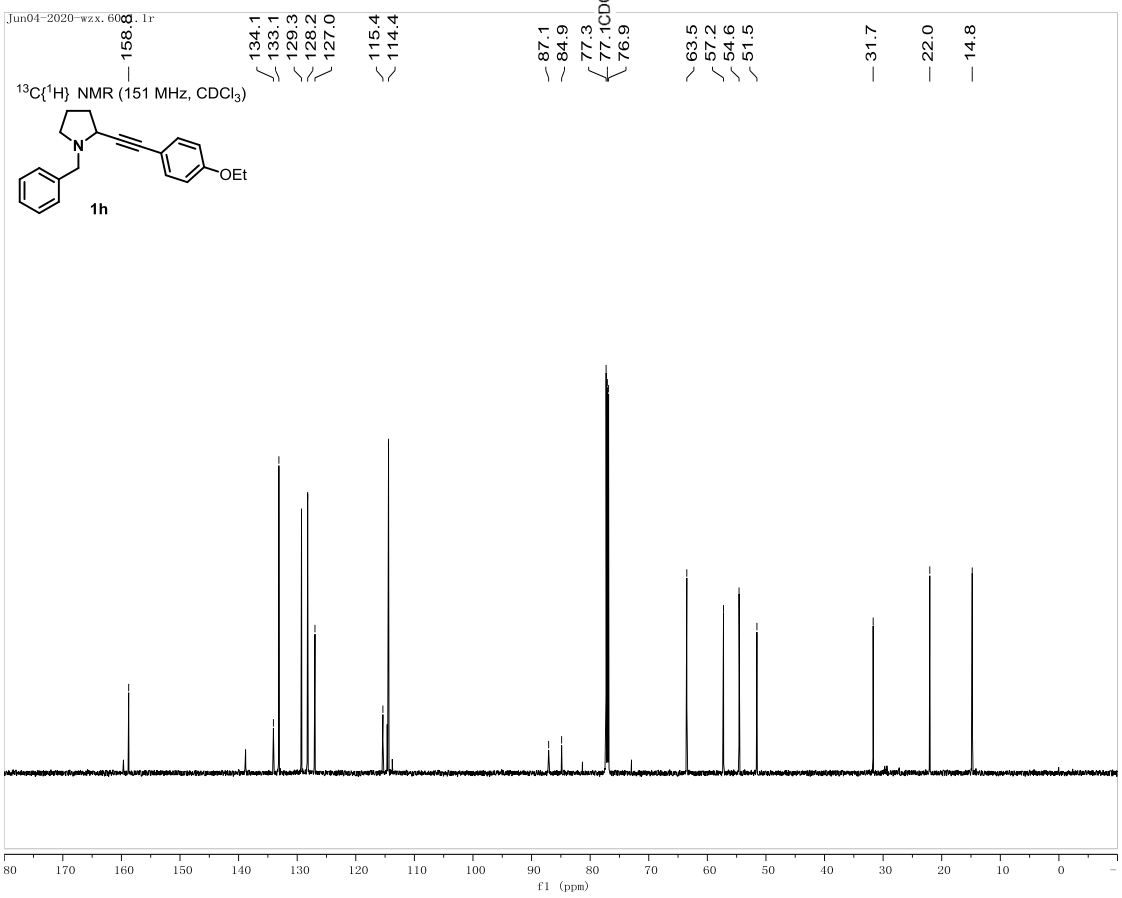

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
1e
f1 (ppm)


^{1}H NMR (400 MHz, $CDCl_3$)
1f
CDCl3
f1 (ppm)


$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
1f
CDCl3
f1 (ppm)


CDCl3
7.46 7.39 7.38 7.37 7.33 7.33 7.32 7.31 7.31 7.30 7.29 7.26 7.24 7.24 7.23 7.22 6.84 6.84 6.83 6.82 4.08 4.05 3.80 3.61 3.57 3.56 3.56 3.54 2.80 2.79 2.77 2.76 2.75 2.54 2.53 2.52 2.51 2.50 2.48 2.15 2.14 2.13 2.13 2.12 2.04 2.03 2.02 2.01 2.01 2.00 1.99 1.92 1.91 1.90 1.80 1.80 1.79 1.78
1H NMR (400 MHz, CDCl3)
N
OMe
1g
4.00 2.00 1.00 2.00 1.00 3.00 2.00 1.00 1.00 2.00 1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


^{1}H NMR (600 MHz, $CDCl_3$)
OEt
1h
f1 (ppm)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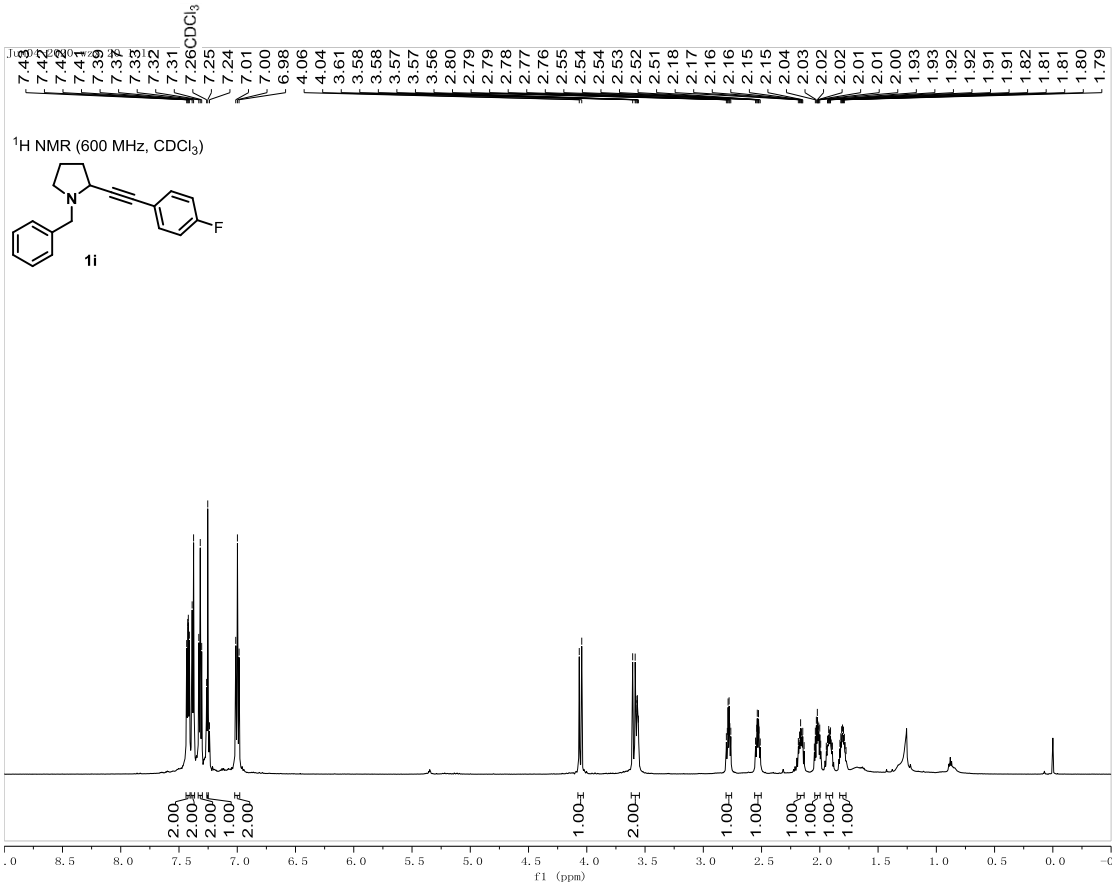
OEt
1h
f1 (ppm)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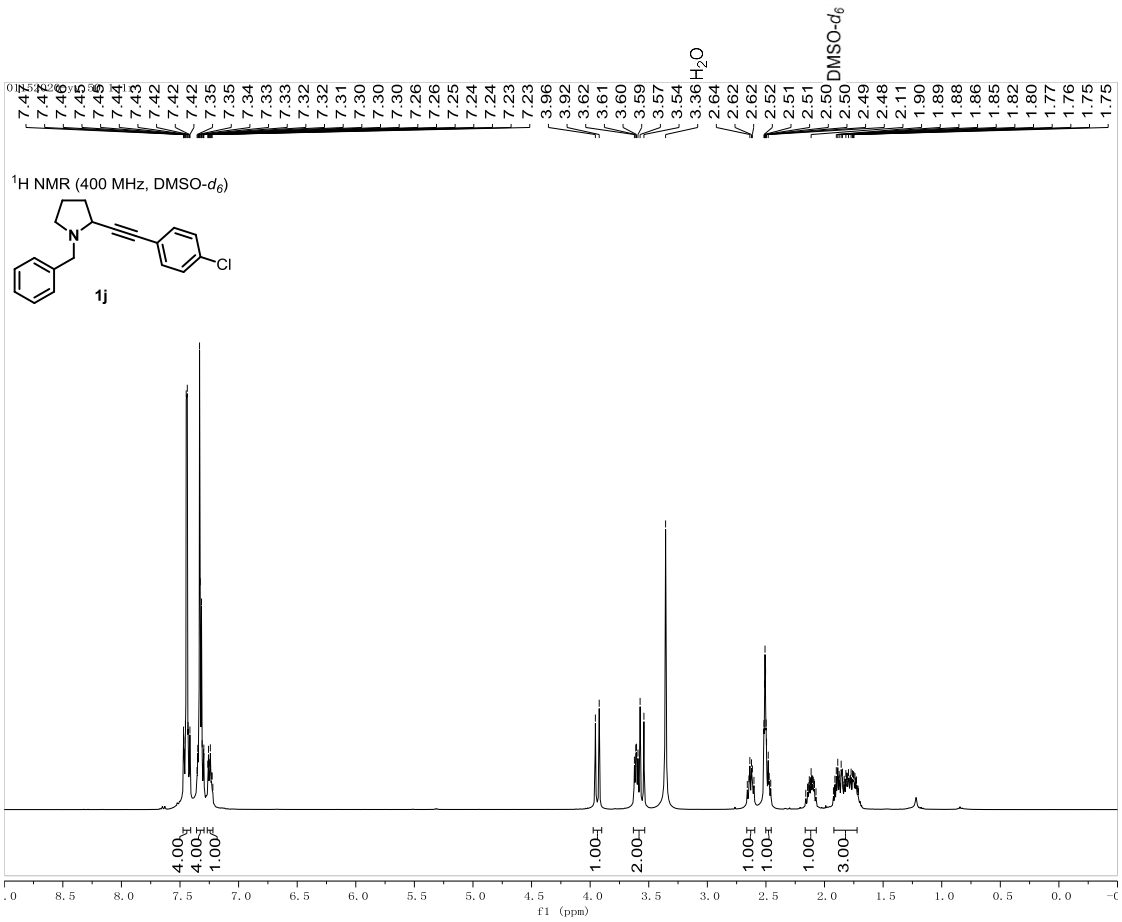
1i
F
$CDCl_3$
f1 (ppm)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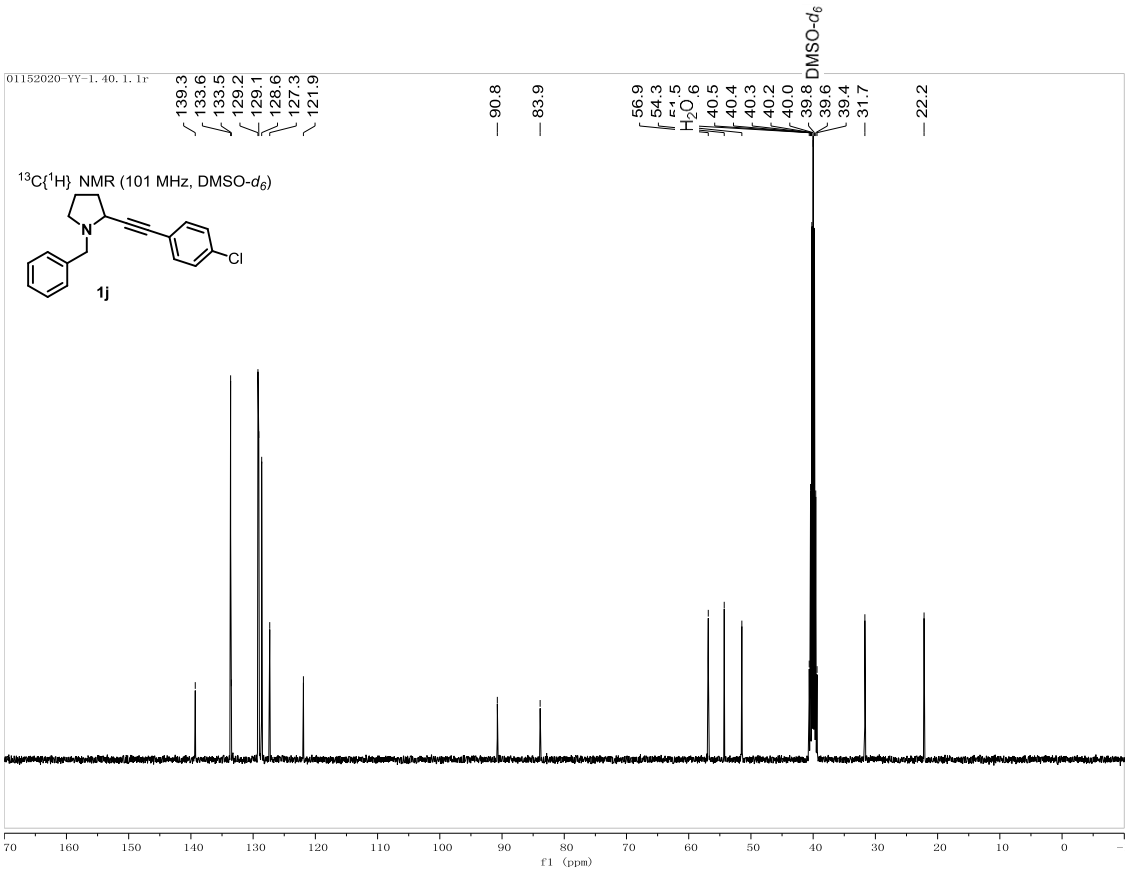
1j
DMSO-d_6
H_2O
f1 (ppm)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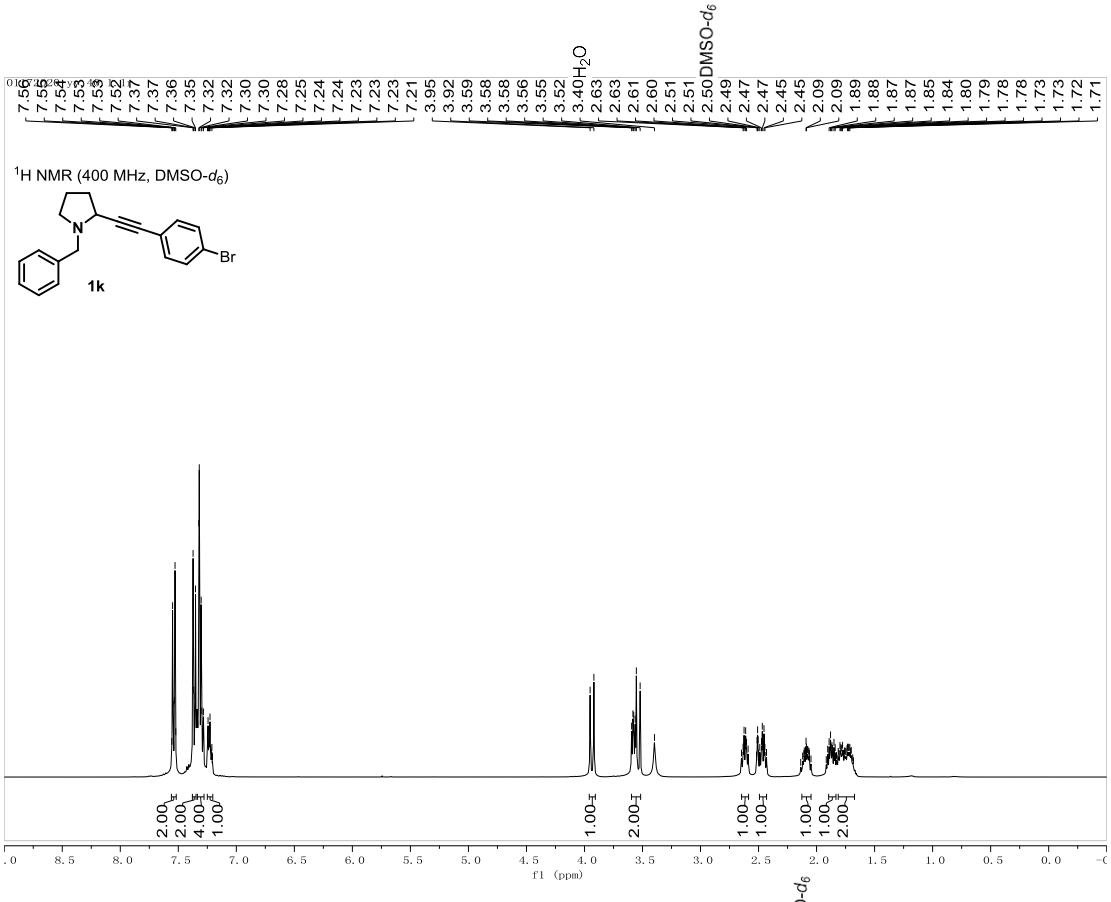
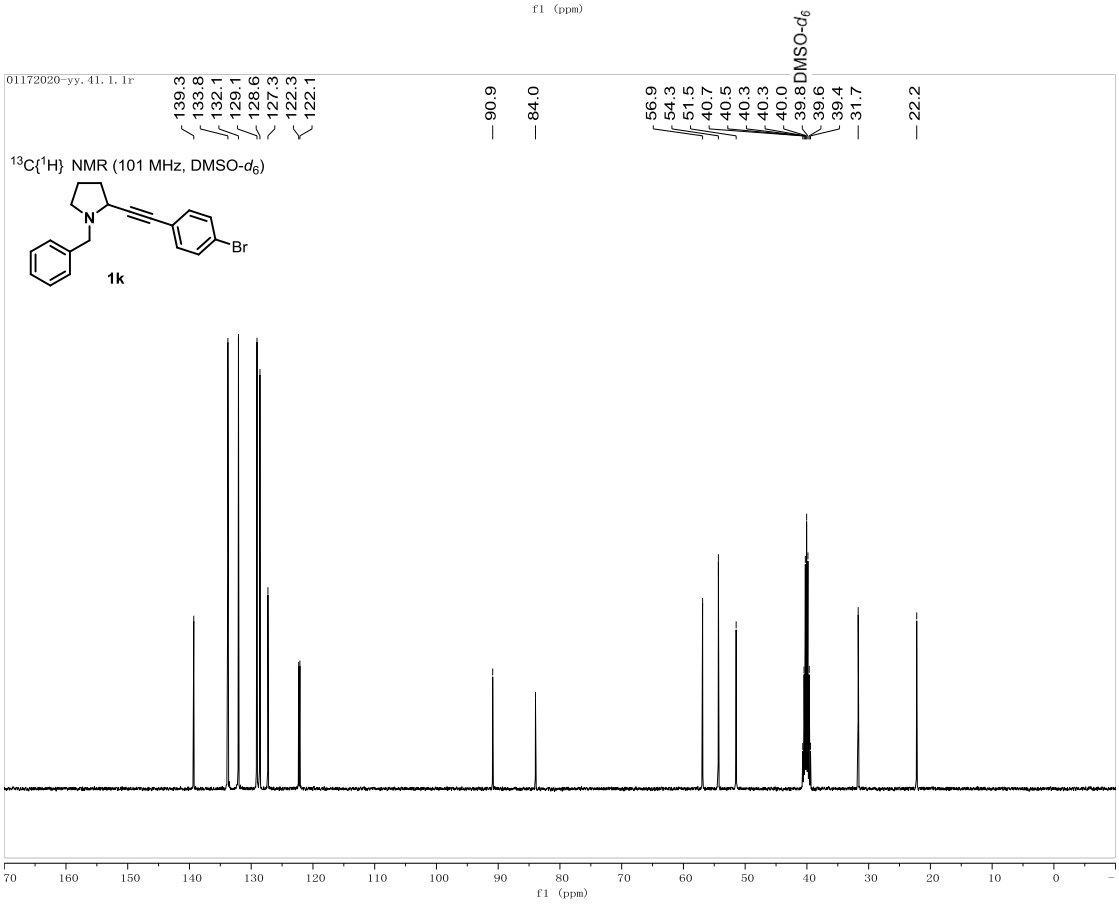
1j
DMSO-d_6
H_2O
f1 (ppm)


^{1}H NMR (400 MHz, DMSO-d_6)
1k
Br
DMSO-d_6
H_2O
f1 (ppm)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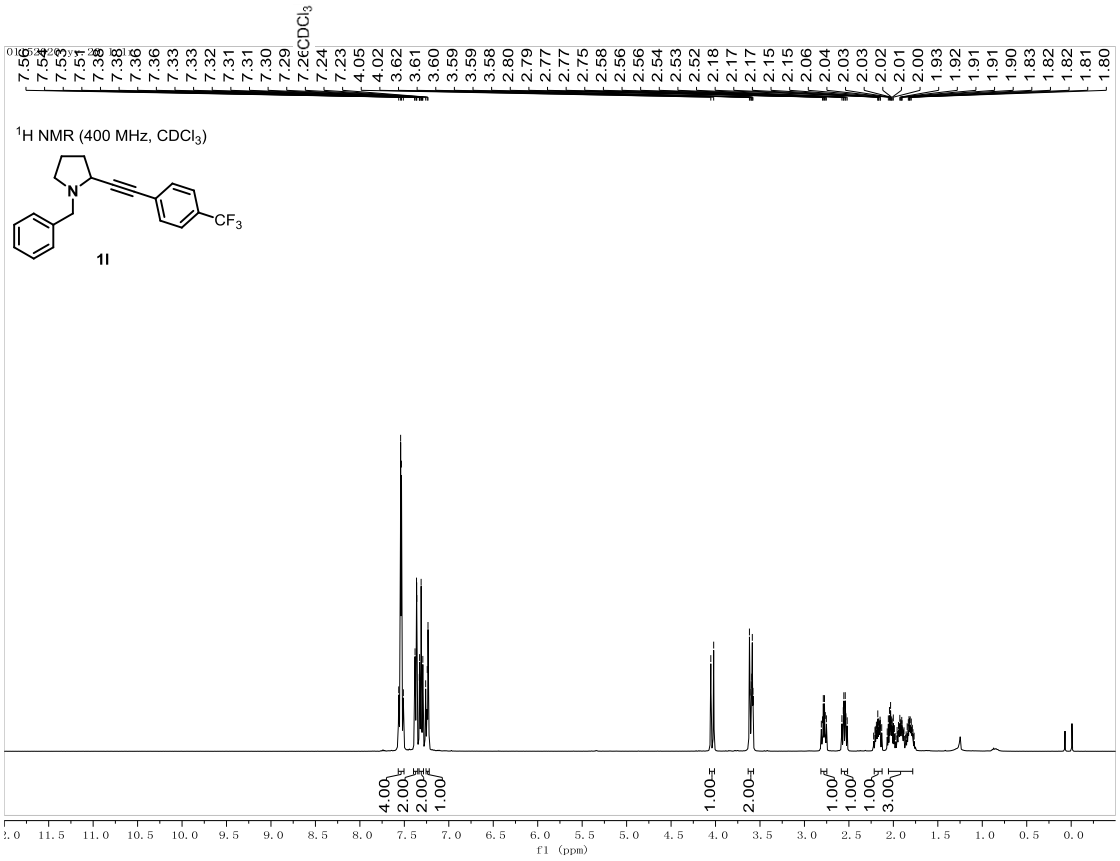
Br
DMSO-d_6
f1 (ppm)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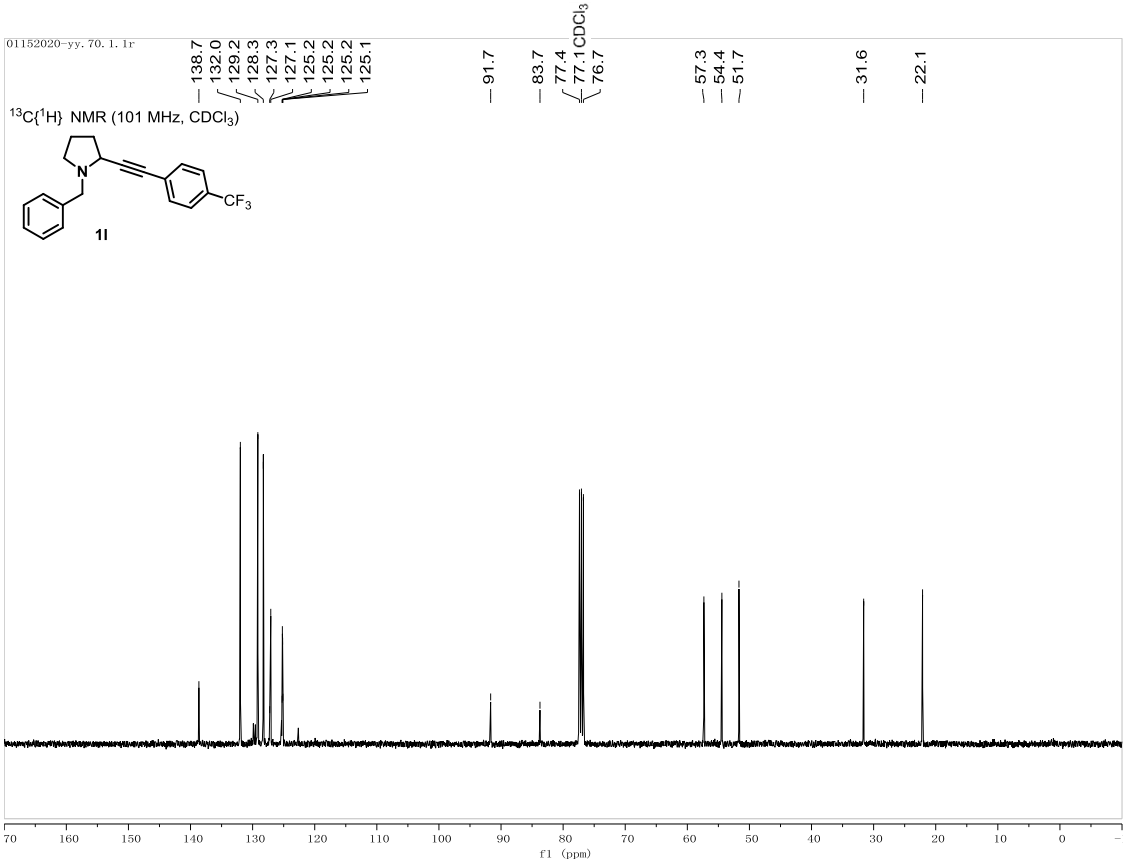
1l
CF$_3$
CDCl$_3$
f1 (ppm)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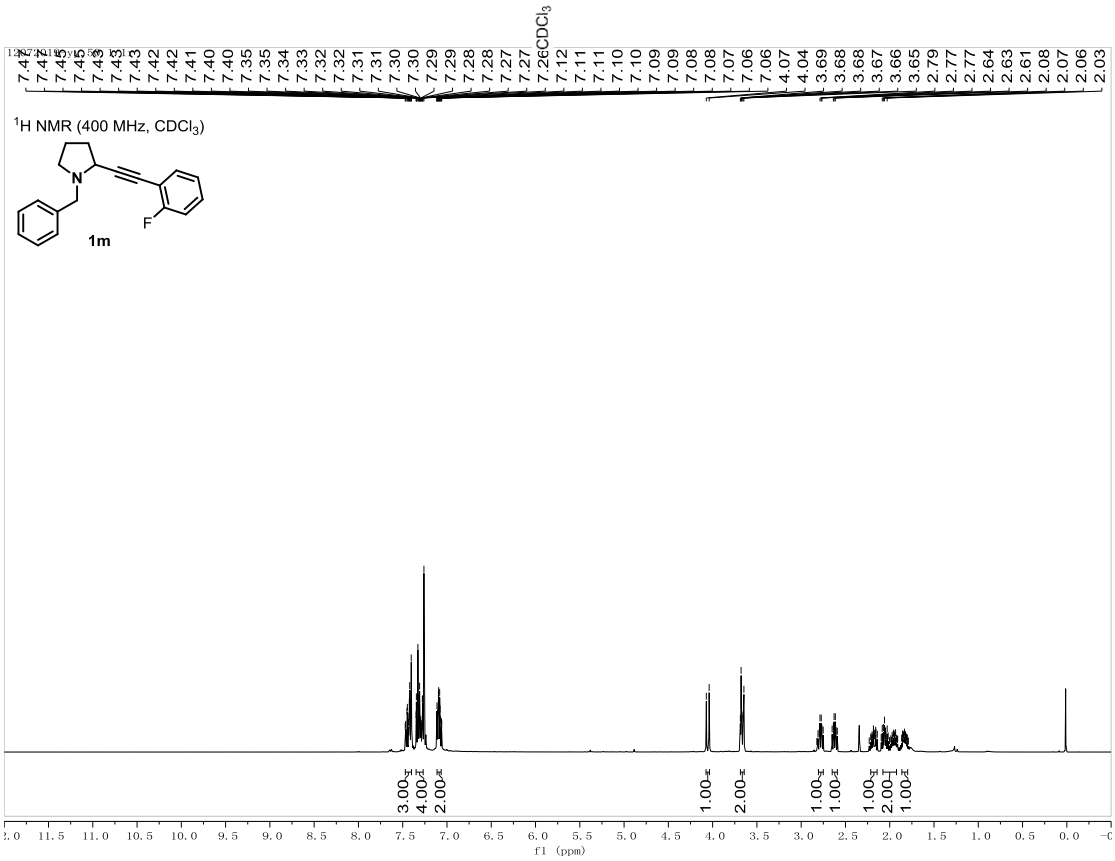
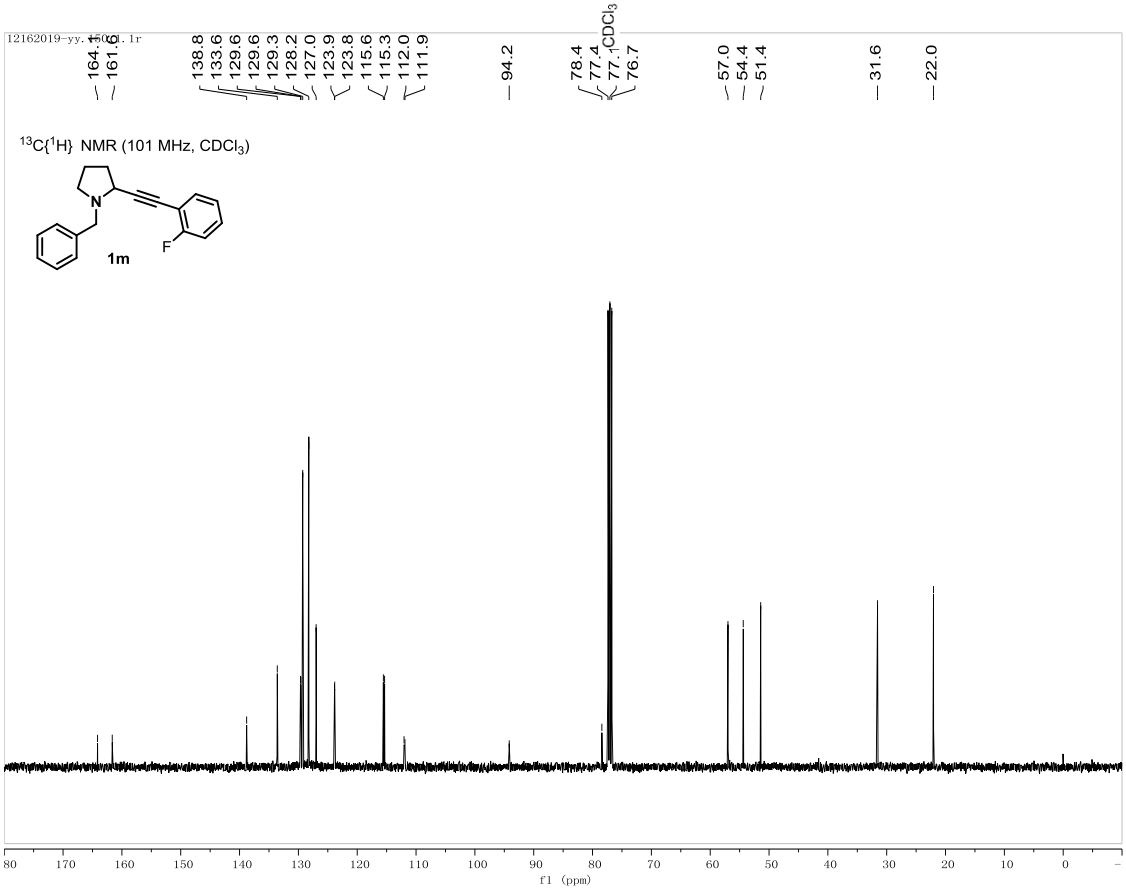
CF$_3$
CDCl$_3$
f1 (ppm)



^{1}H NMR (400 MHz, $CDCl_3$)
1m
f1 (ppm)



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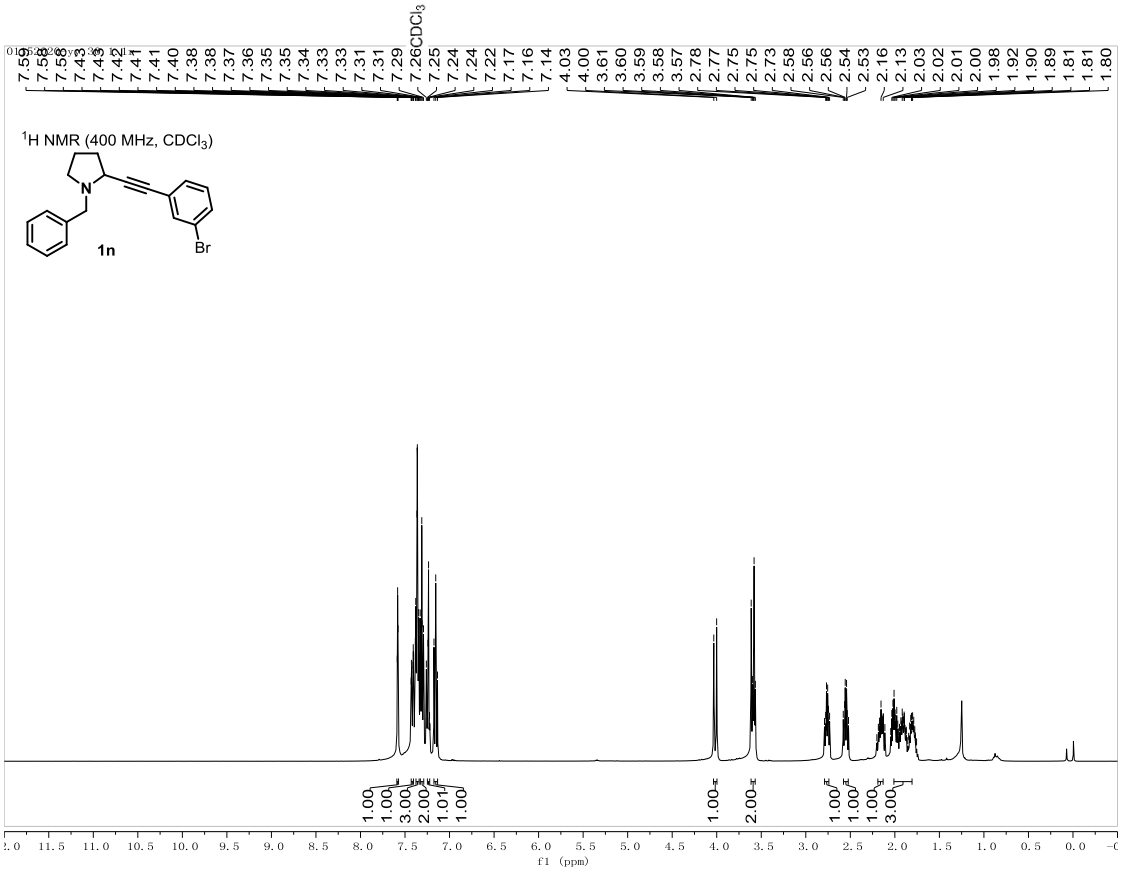
1m
f1 (ppm)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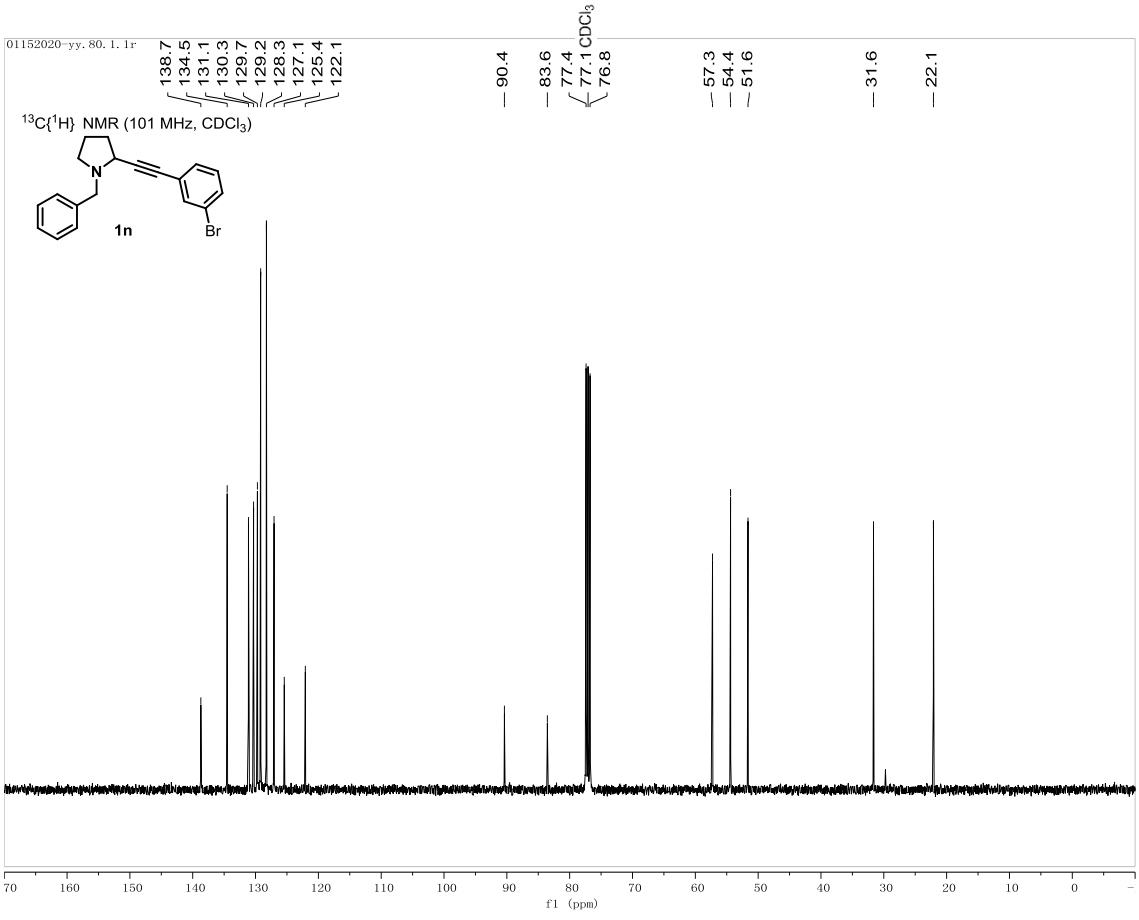
1n
Br
f1 (ppm)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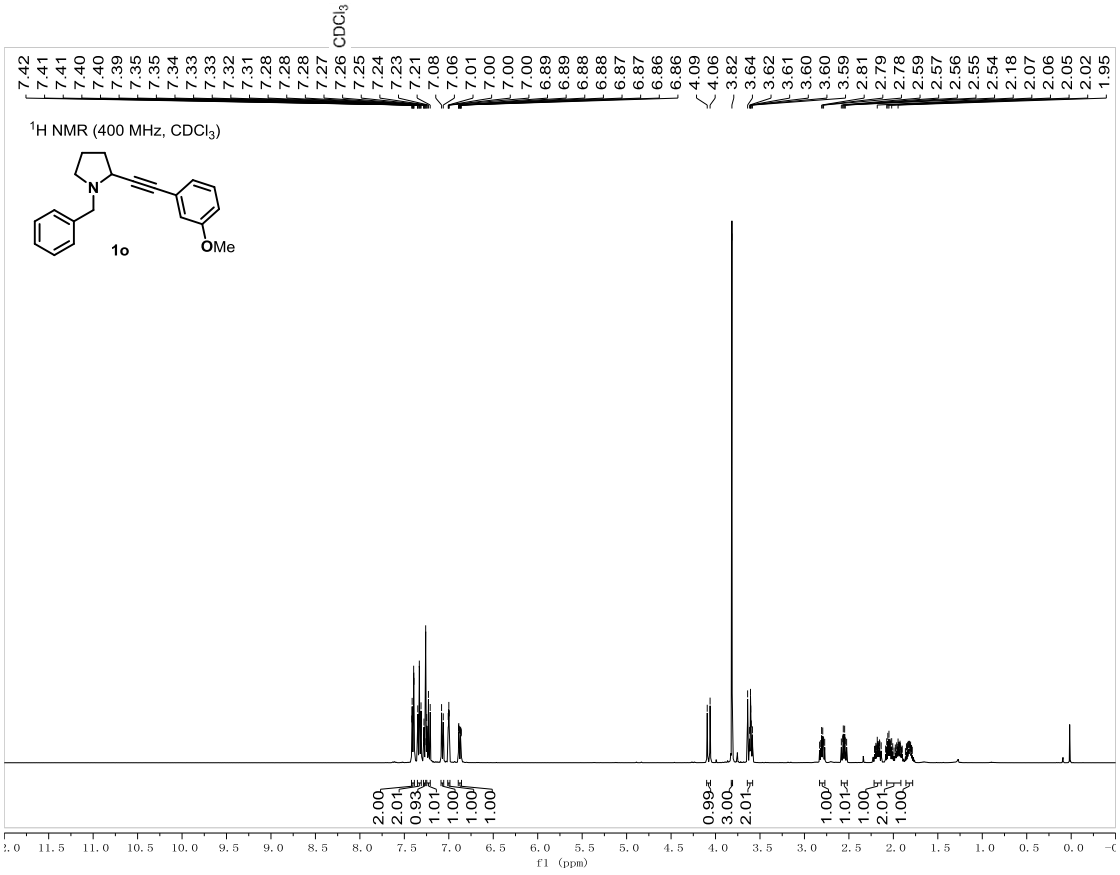
Br
f1 (ppm)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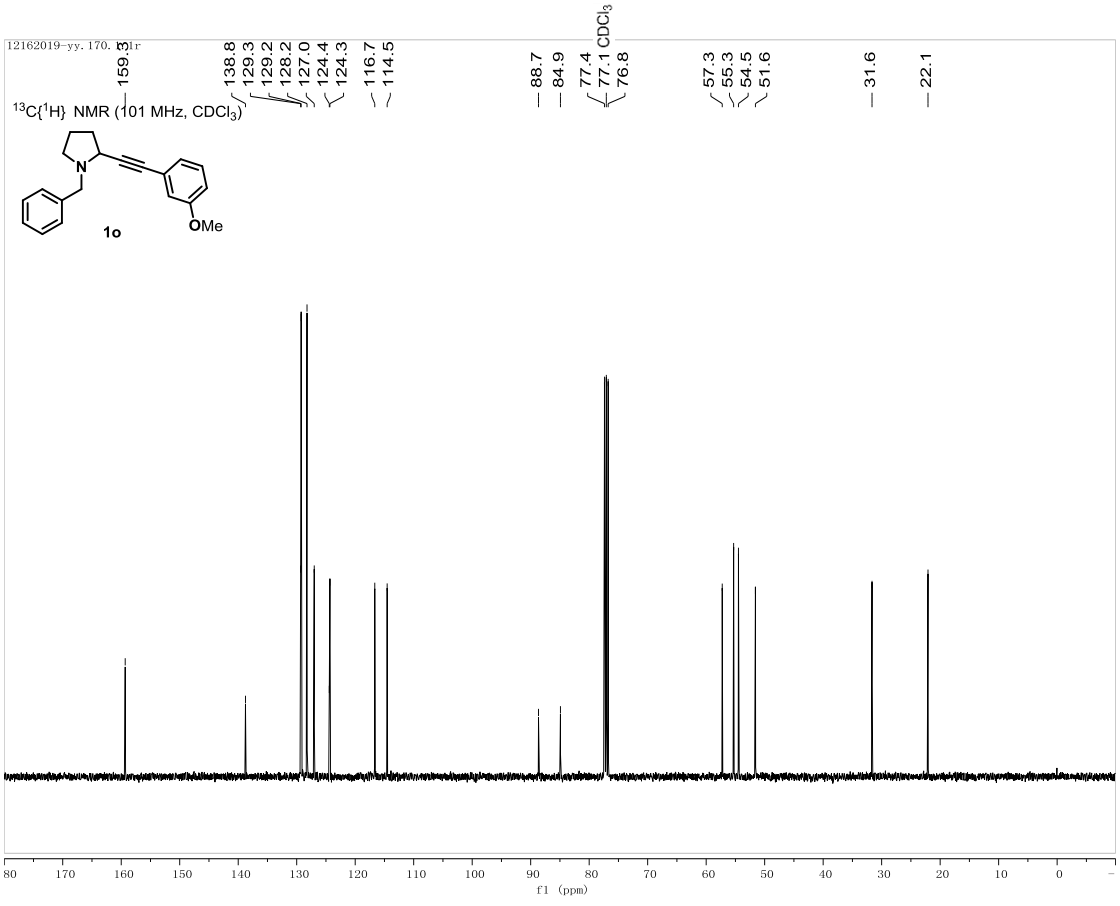
1o
OMe
CDCl3
f1 (ppm)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1o
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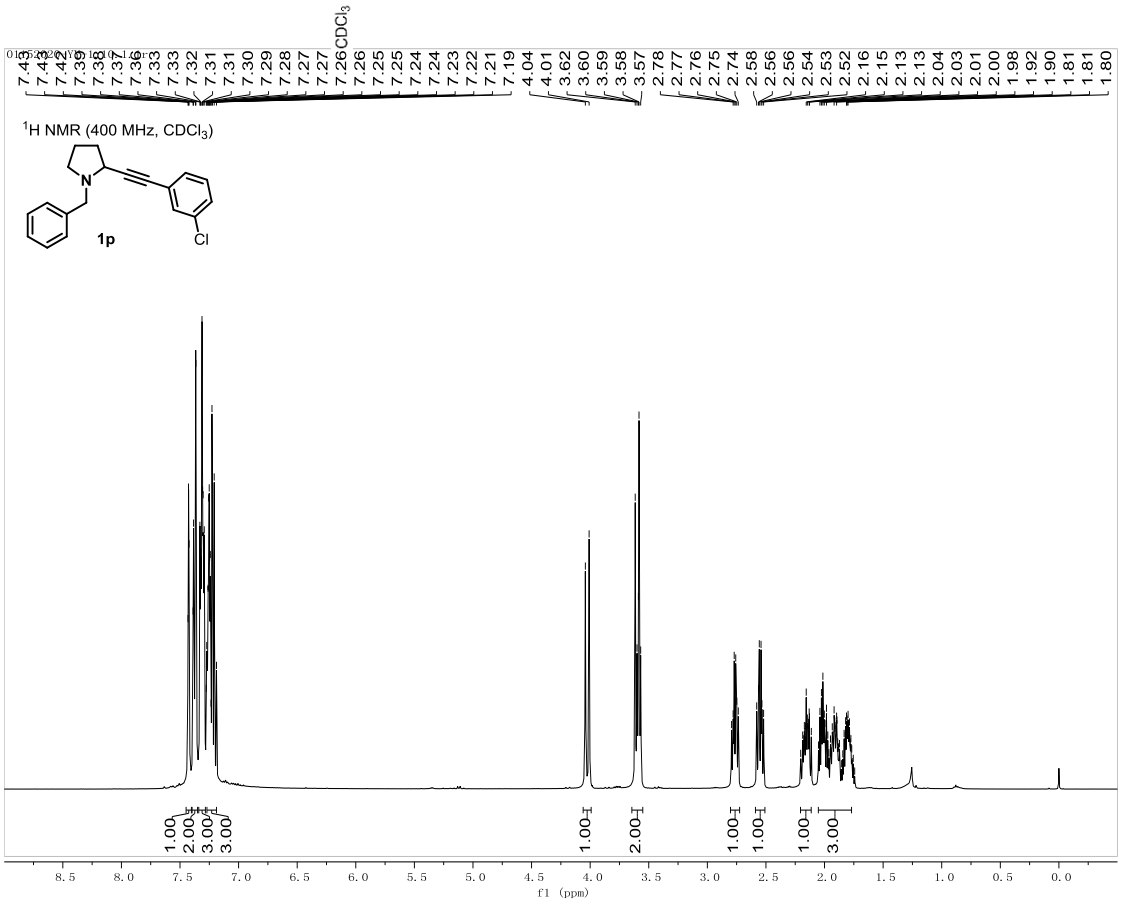
CDCl3
f1 (ppm)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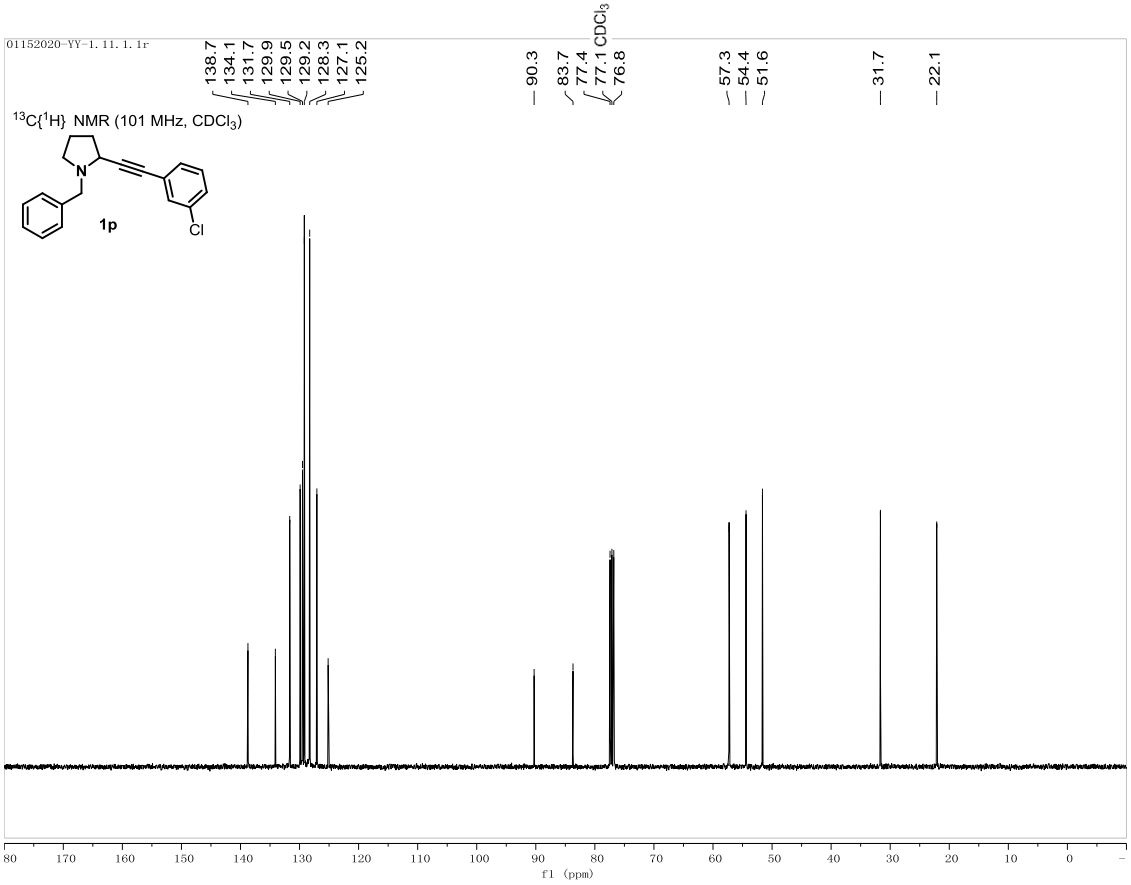
1p
Cl
$CDCl_3$
f1 (ppm)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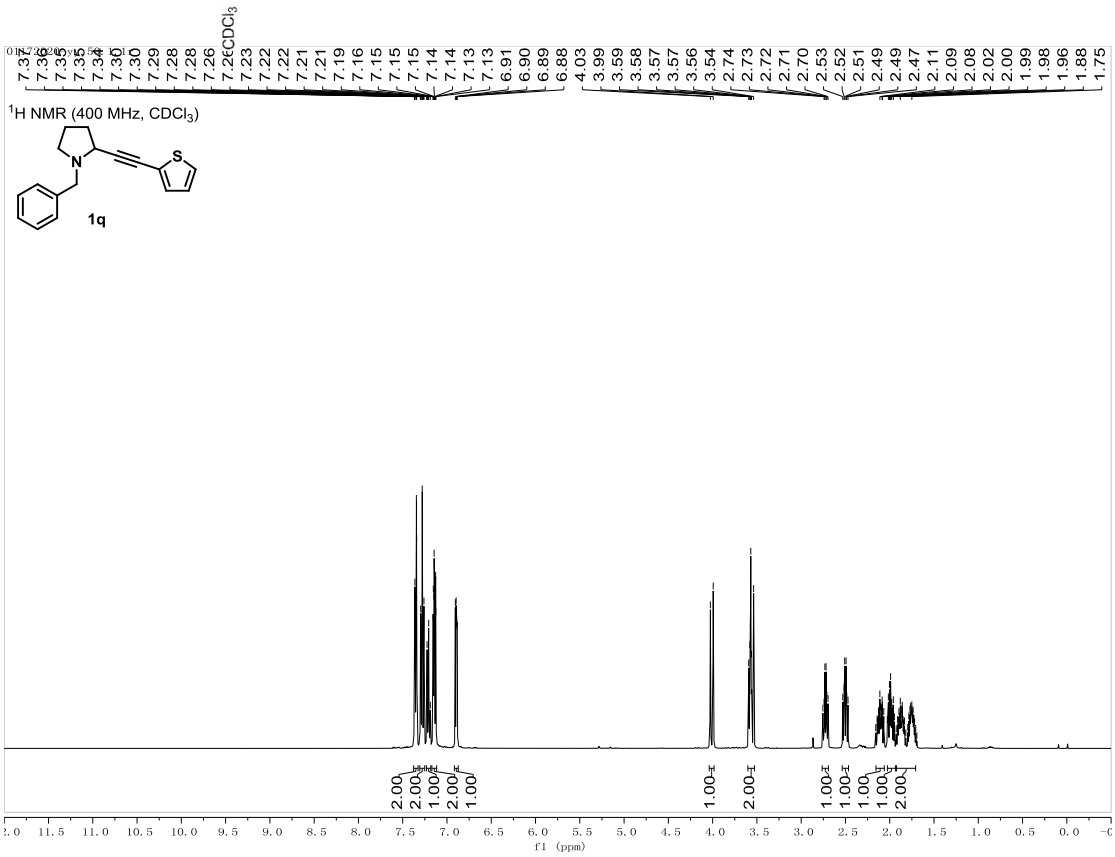
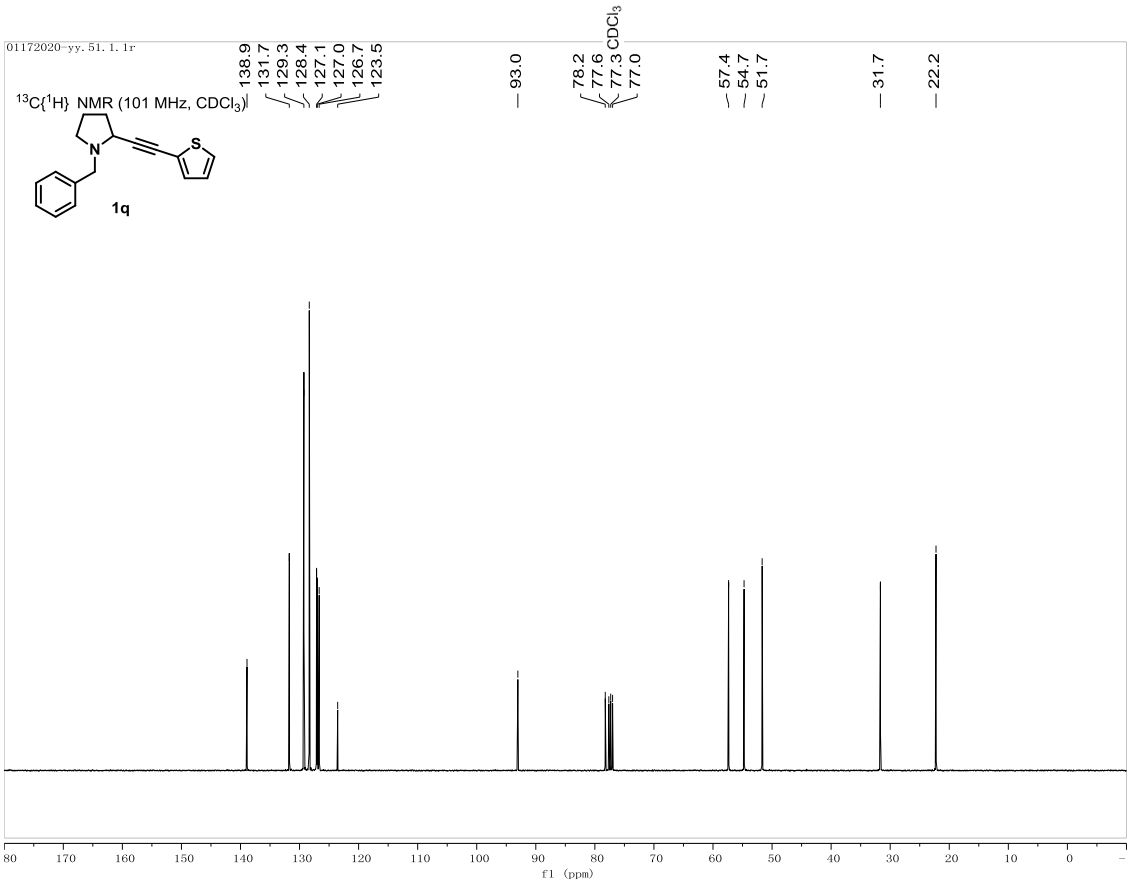
1p
Cl
$CDCl_3$
f1 (ppm)


^{1}H NMR (400 MHz, $CDCl_3$)
1q
f1 (ppm)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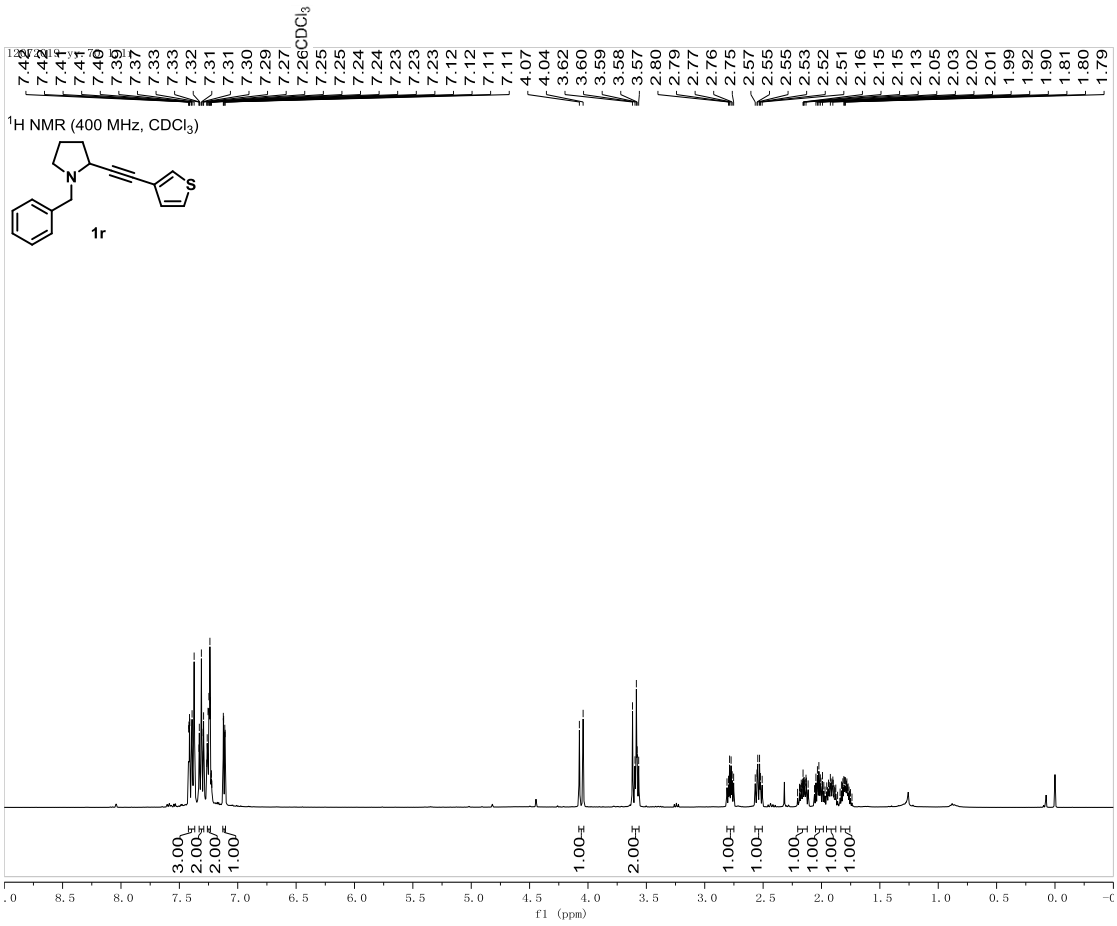
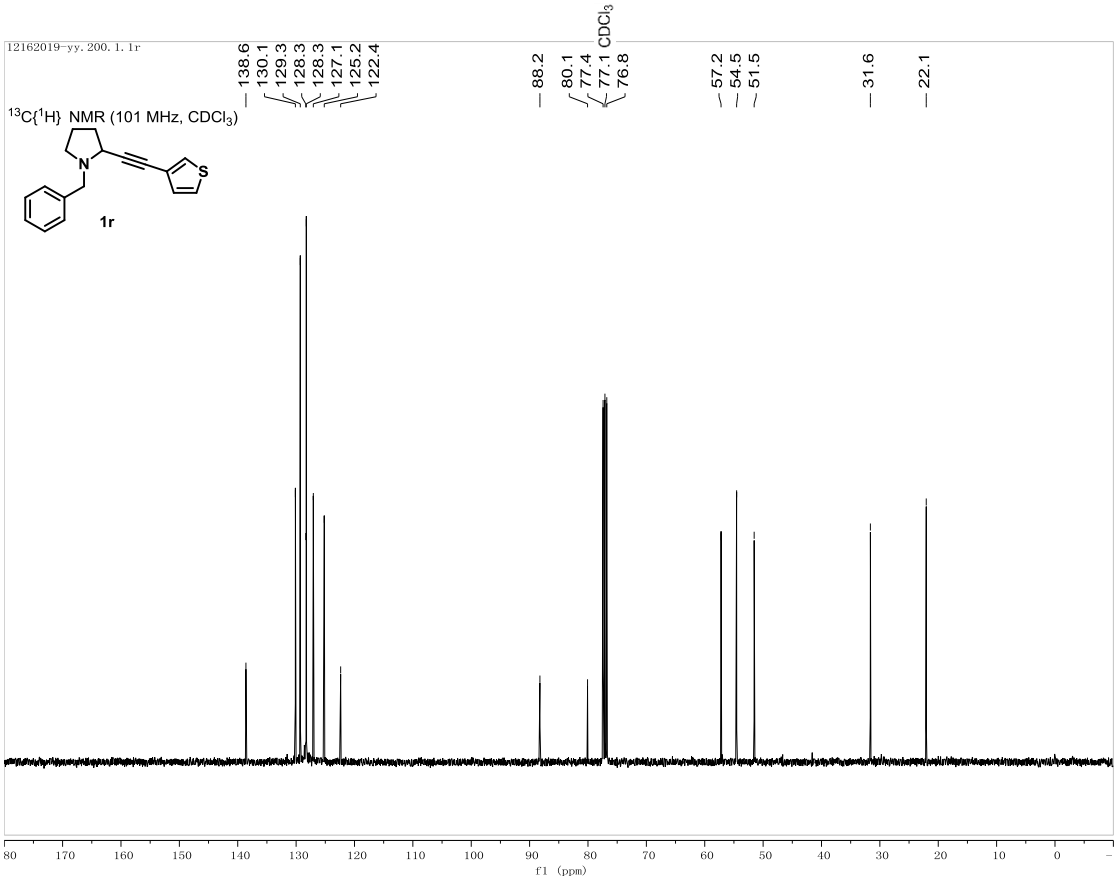
1q
f1 (ppm)


^{1}H NMR (400 MHz, $CDCl_3$)
1r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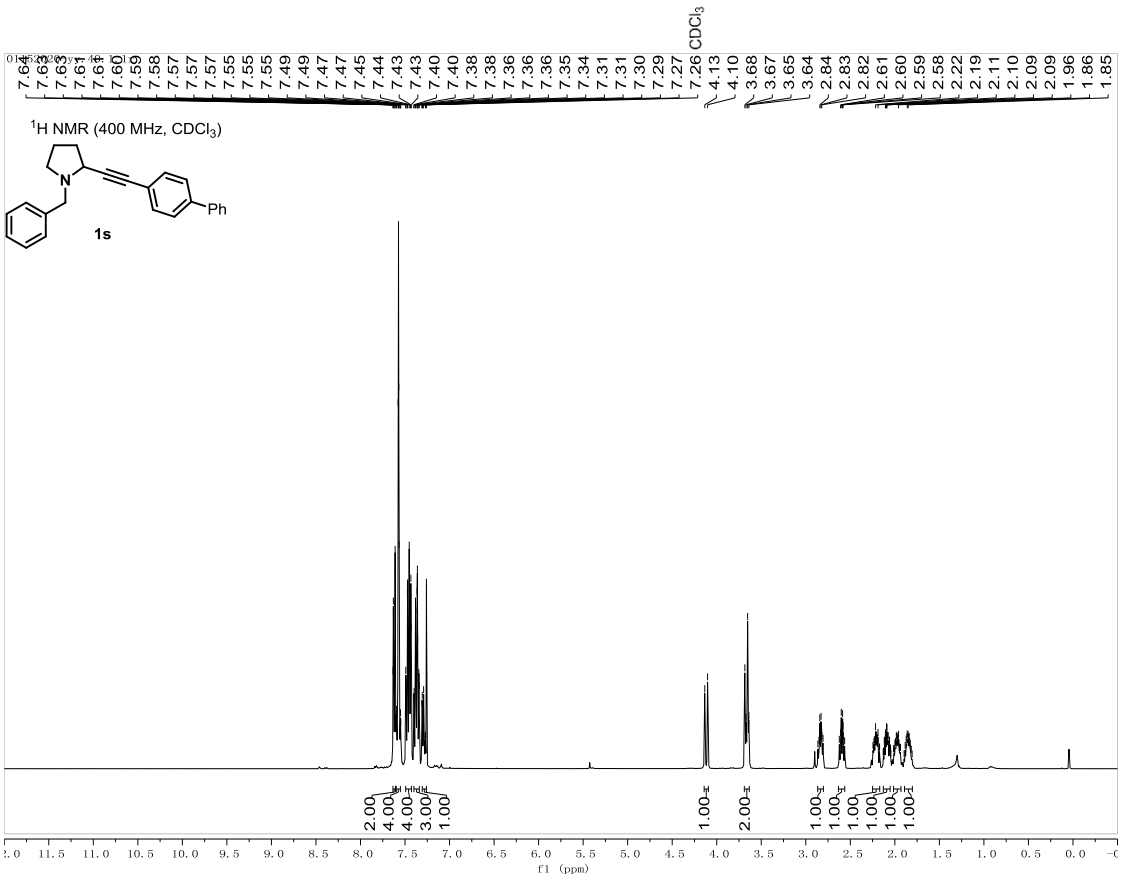
1r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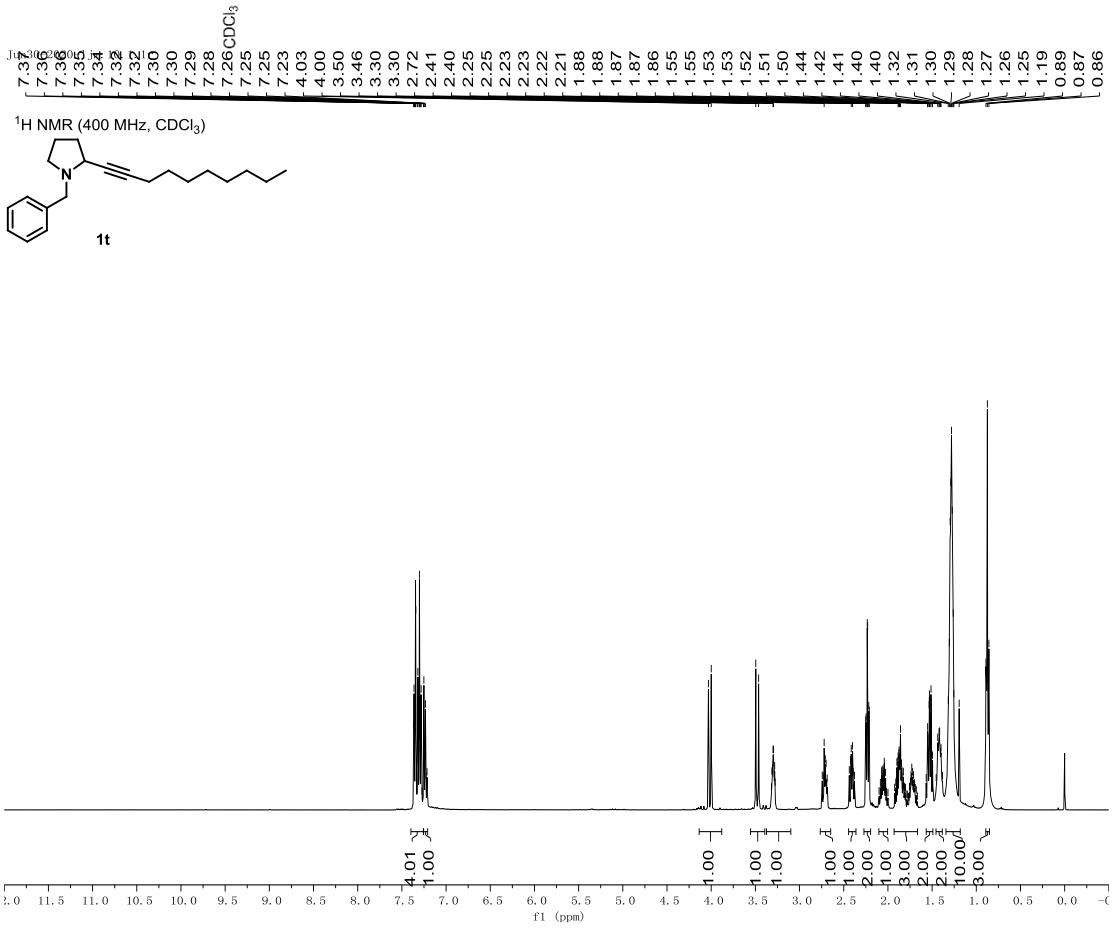
Ph
1s
$CDCl_3$
f1 (ppm)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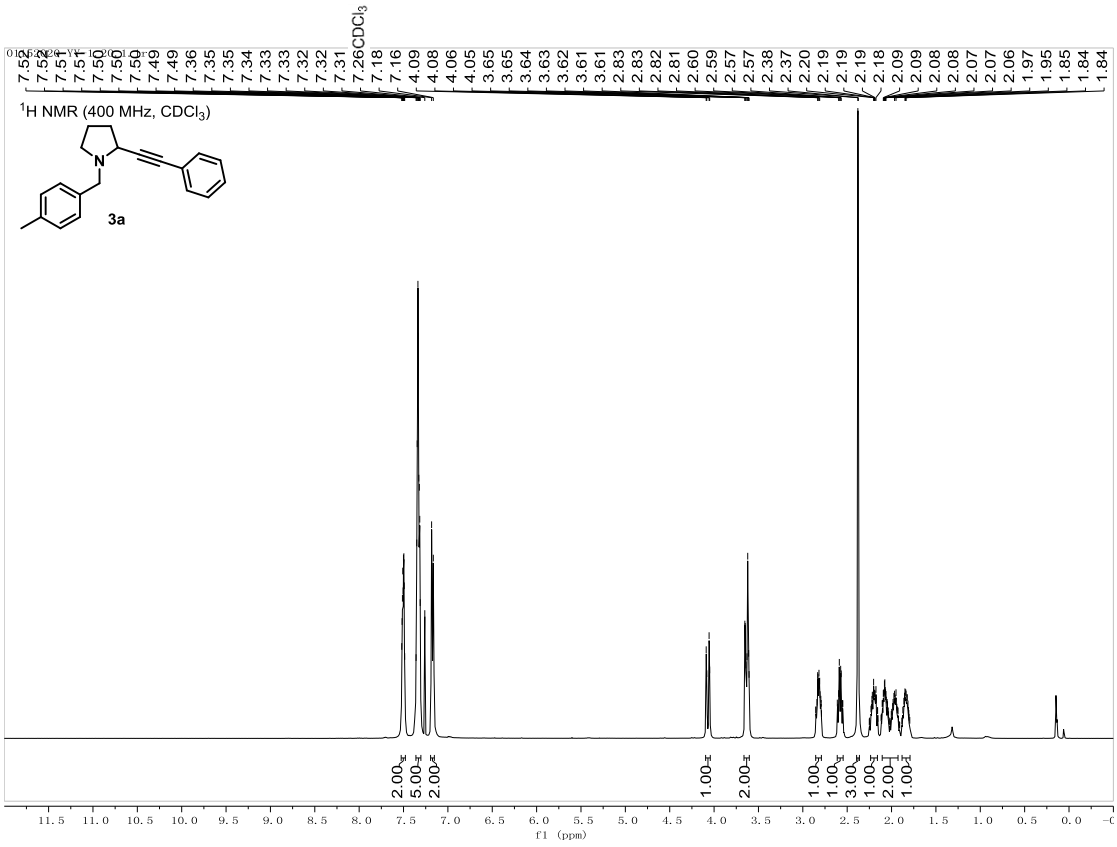
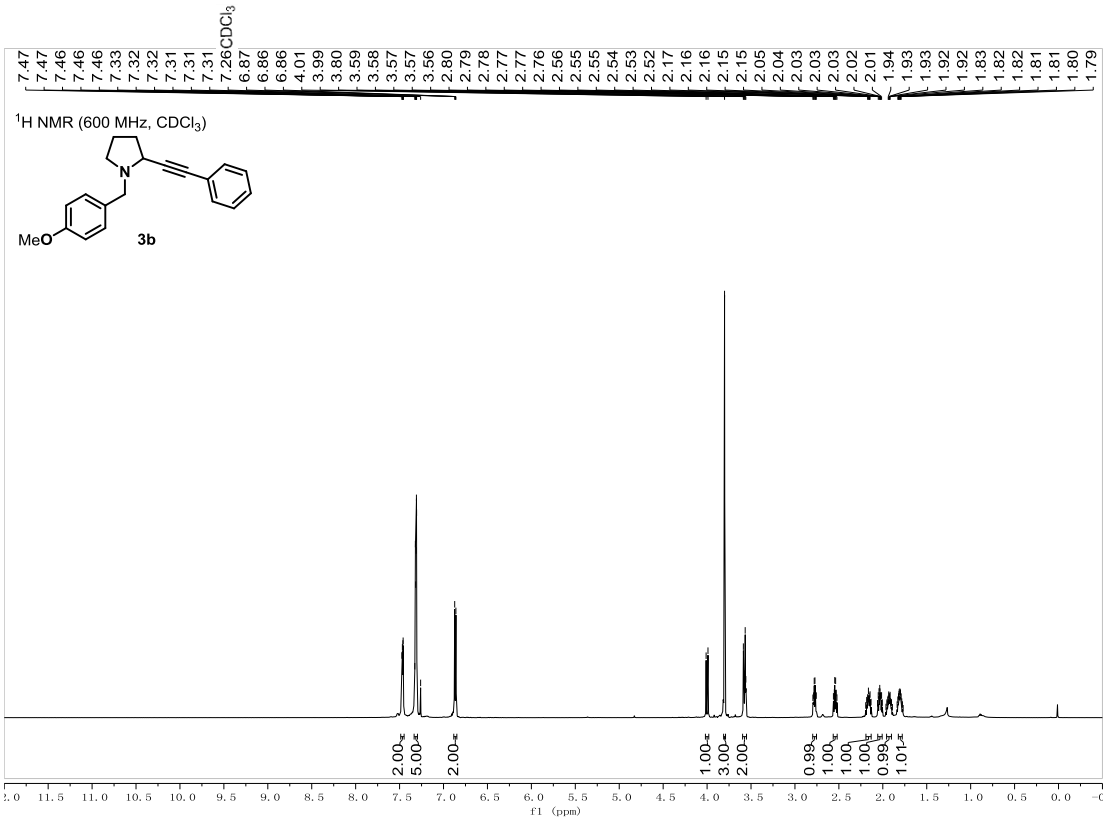
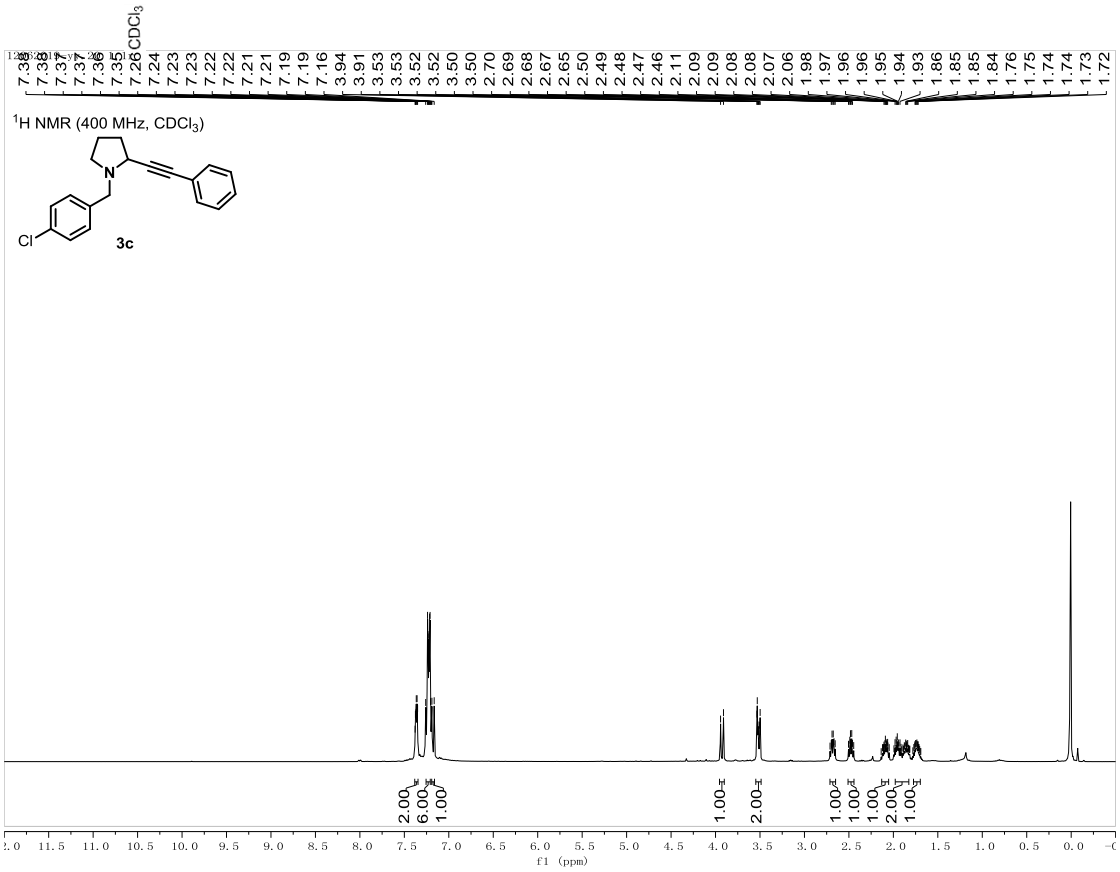
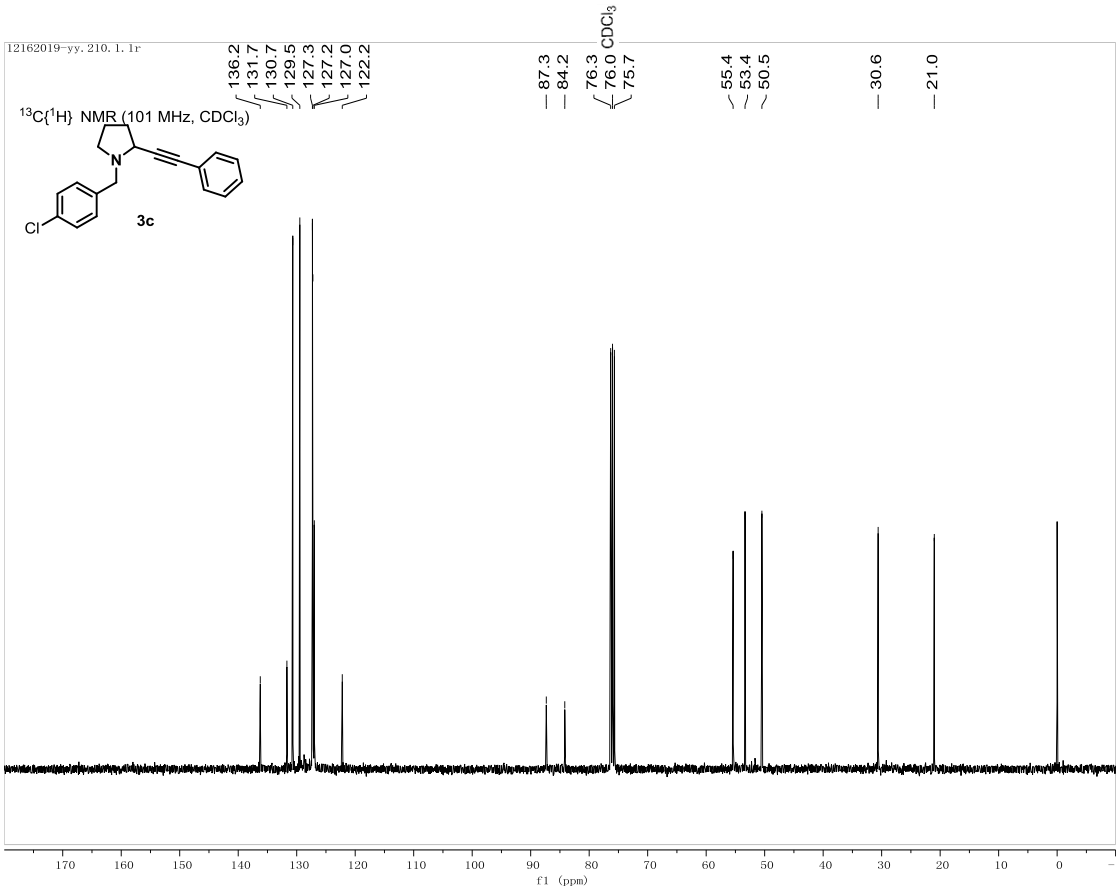
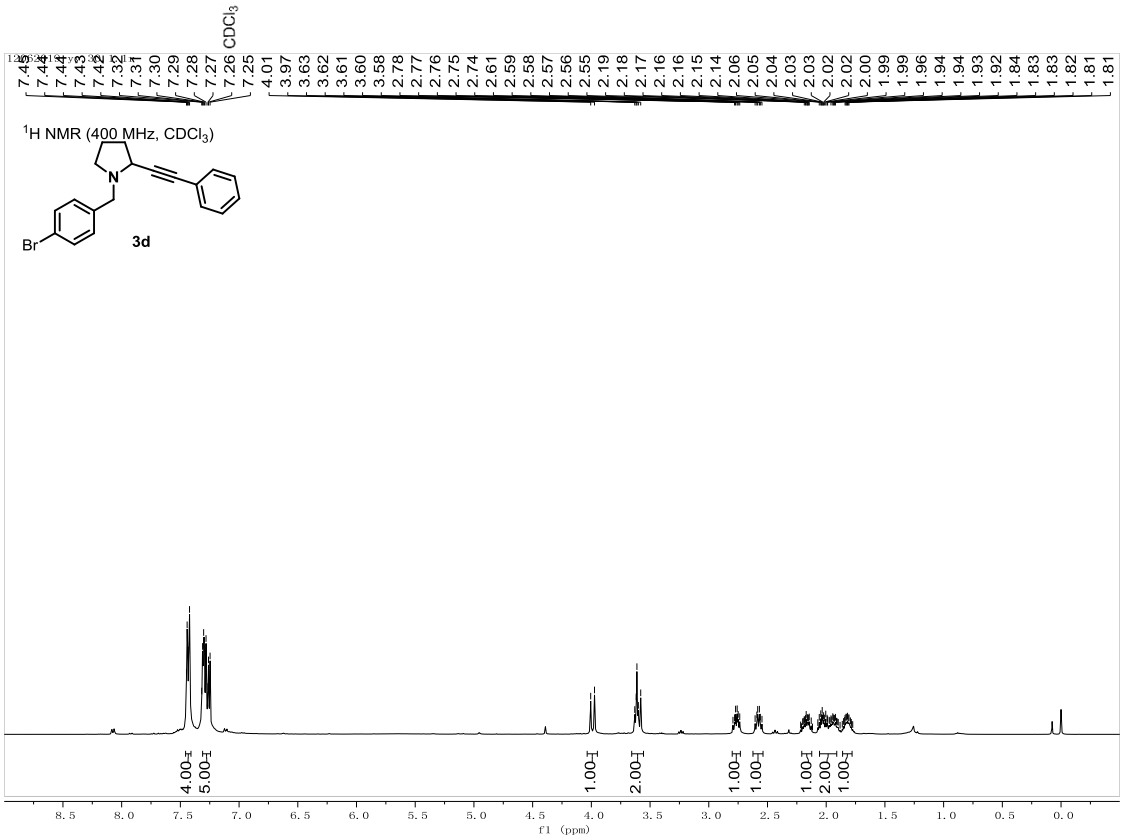
1H NMR (400 MHz, CDCl3)
N
1t
4.01 1.00 1.00 1.00 1.00 1.00 1.00 2.00 1.00 3.00 2.00 2.00 10.00 3.00
f1 (ppm)

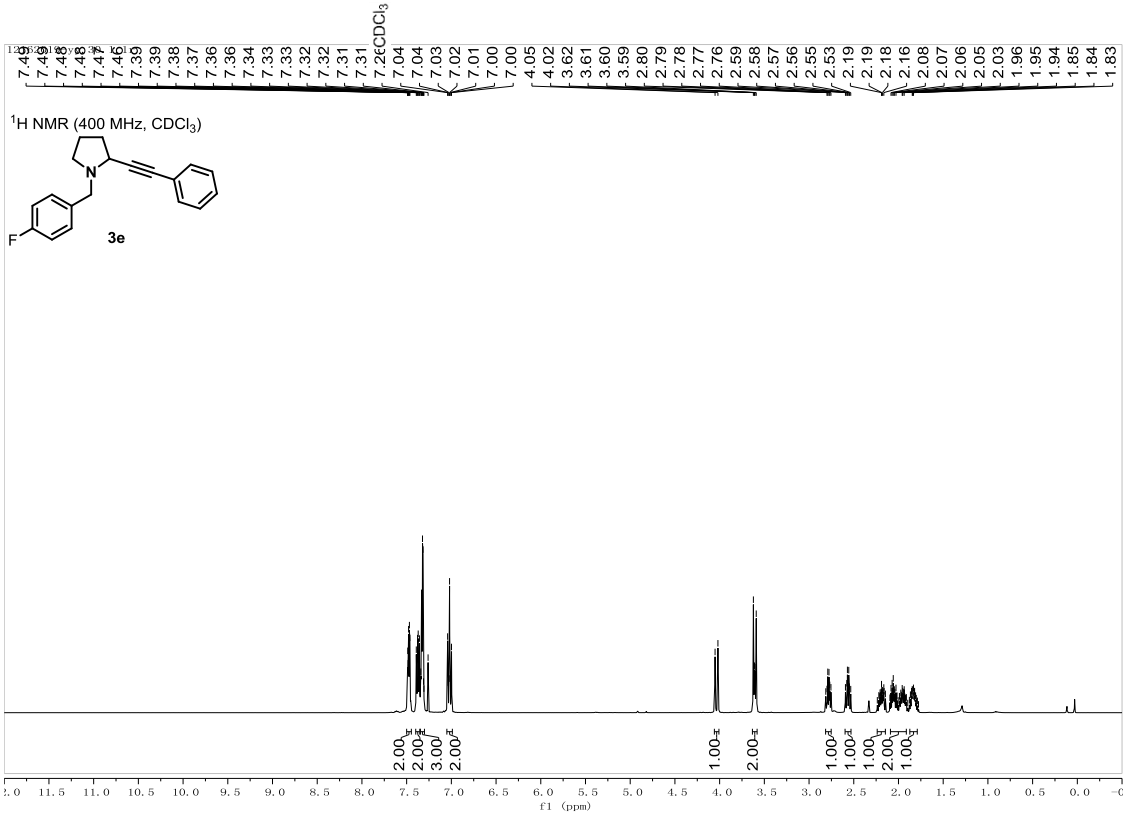

^{1}H NMR (400 MHz, $CDCl_3$)
3a
$CDCl_3$
f1 (ppm)

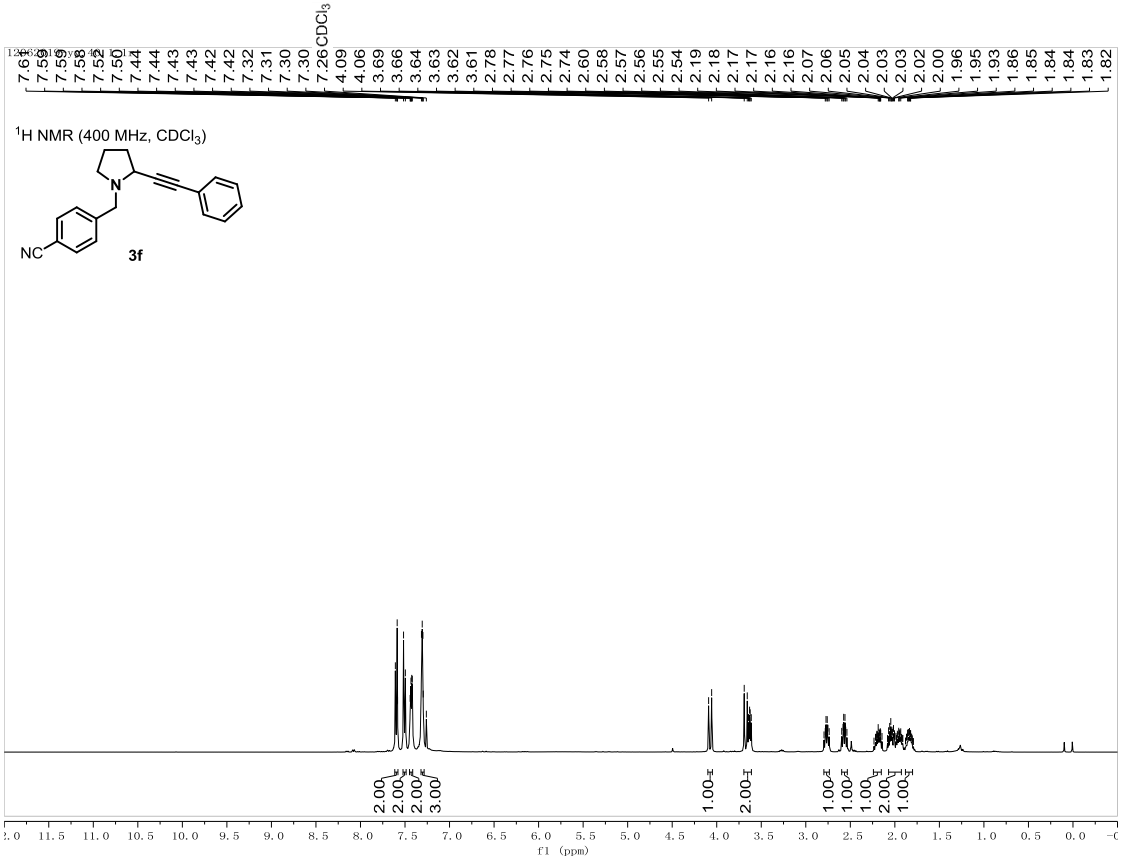

^{1}H NMR (600 MHz, $CDCl_3$)
MeO
3b
f1 (ppm)

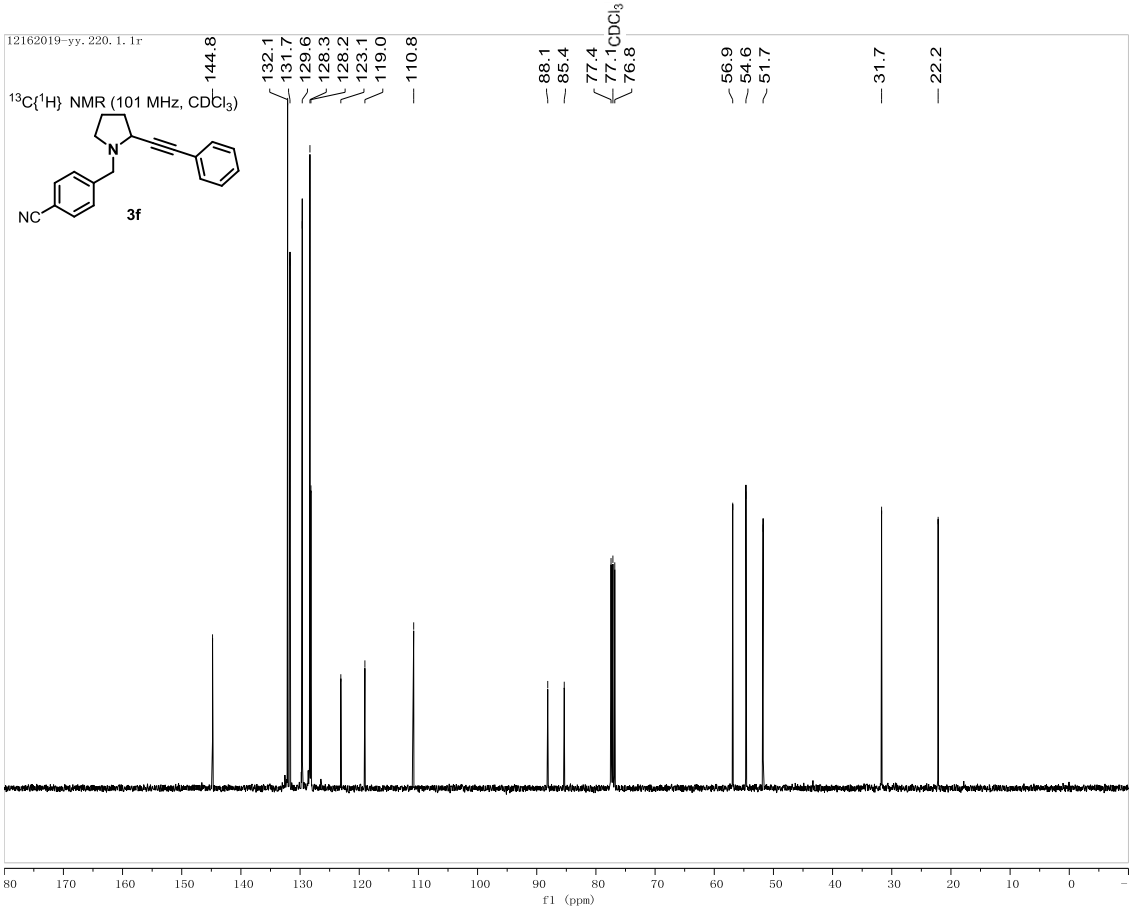

^{1}H NMR (400 MHz, CDCl$_3$)
3c
CDCl$_3$
f1 (ppm)

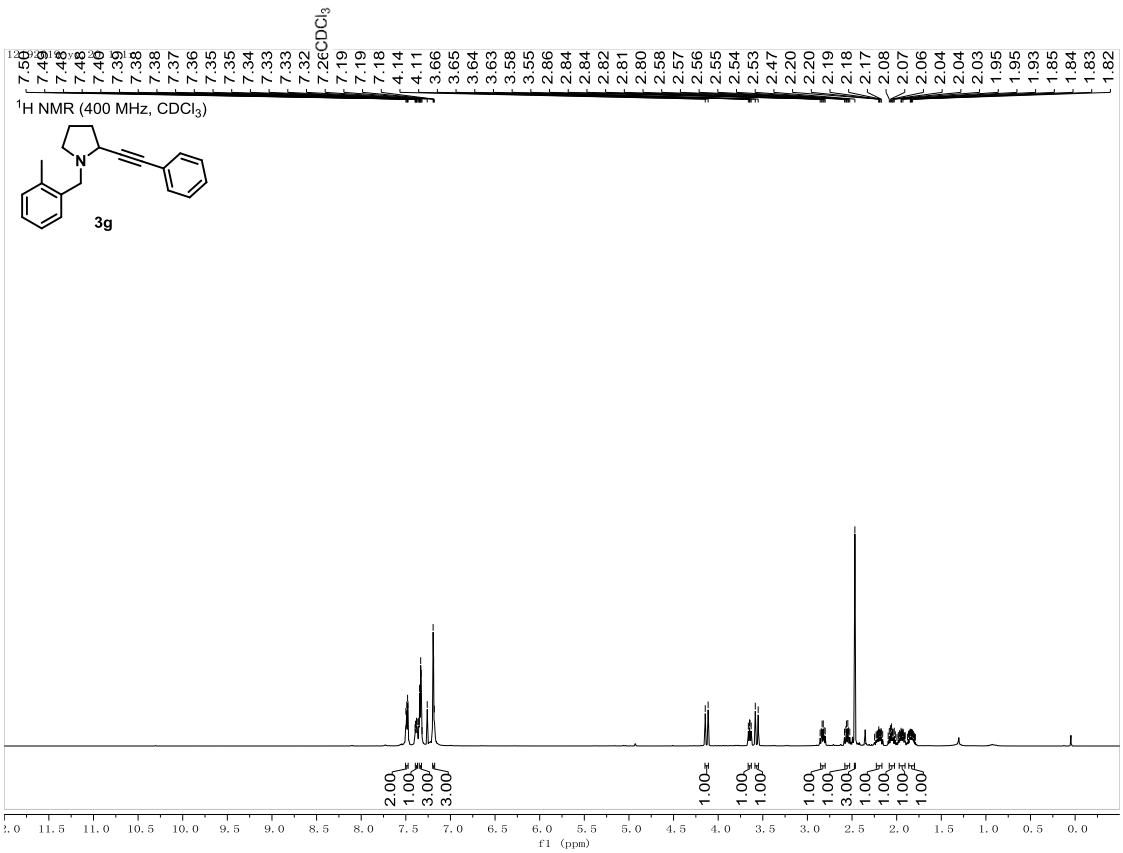

^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)
3c
CDCl$_3$
f1 (ppm)

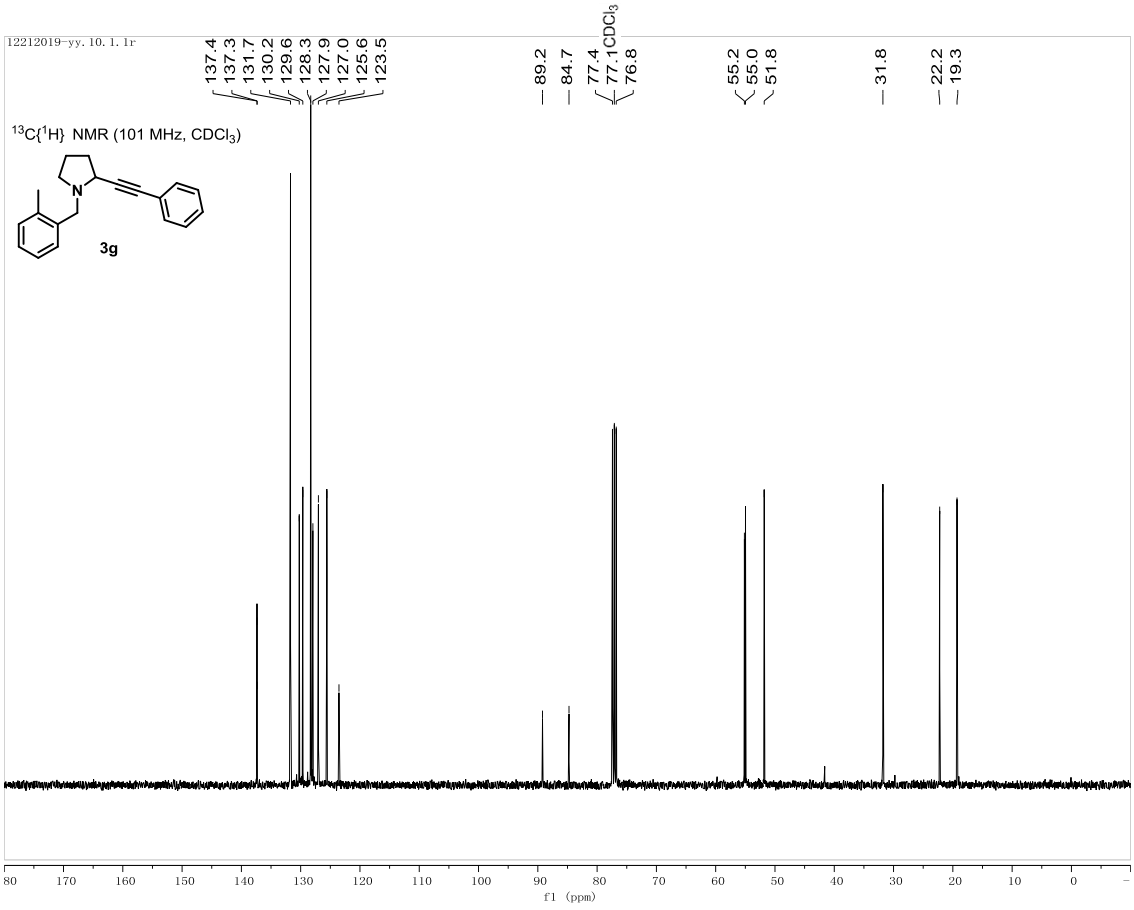

^{1}H NMR (400 MHz, $CDCl_3$)
Br
3d
$CDCl_3$
7.45 7.44 7.44 7.43 7.43 7.42 7.32 7.31 7.30 7.29 7.28 7.27 7.26 7.25
4.01 3.97 3.63 3.62 3.61 3.60 3.58 2.78 2.77 2.76 2.75 2.74 2.61 2.59 2.58 2.57 2.56 2.55 2.19 2.18 2.17 2.16 2.16 2.15 2.14 2.06 2.05 2.04 2.03 2.03 2.02 2.02 2.00 1.99 1.99 1.96 1.94 1.94 1.93 1.92 1.84 1.83 1.83 1.82 1.81 1.81
4.00 5.00 1.00 2.00 1.00 1.00 1.00 2.00 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

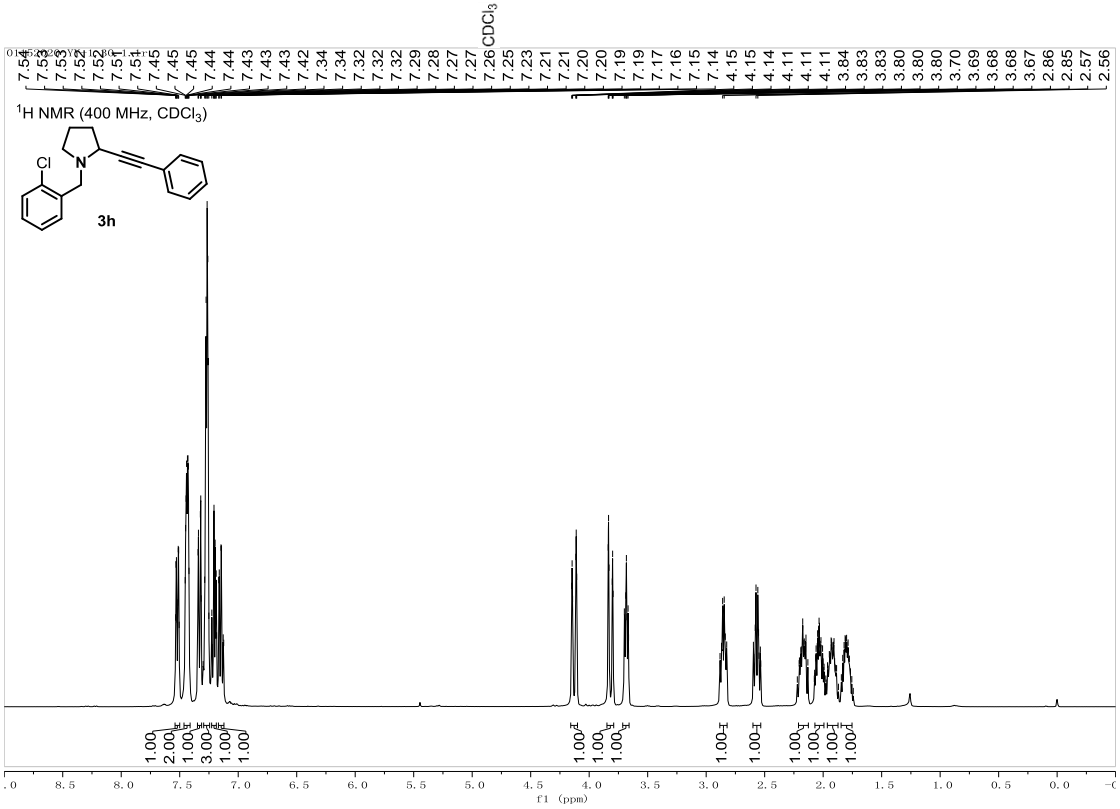

^{1}H NMR (400 MHz, CDCl$_3$)
3e
CDCl$_3$
f1 (ppm)

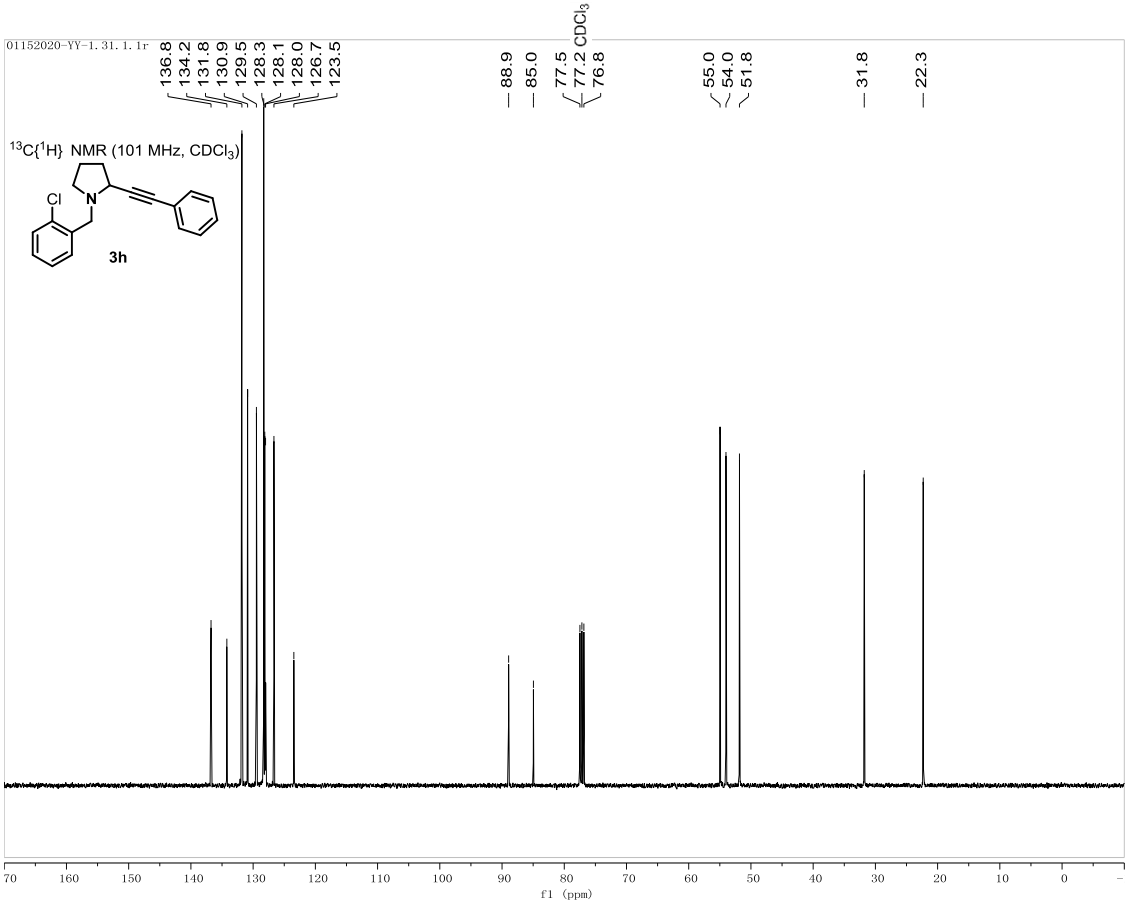

^{1}H NMR (400 MHz, $CDCl_3$)
3f
f1 (ppm)

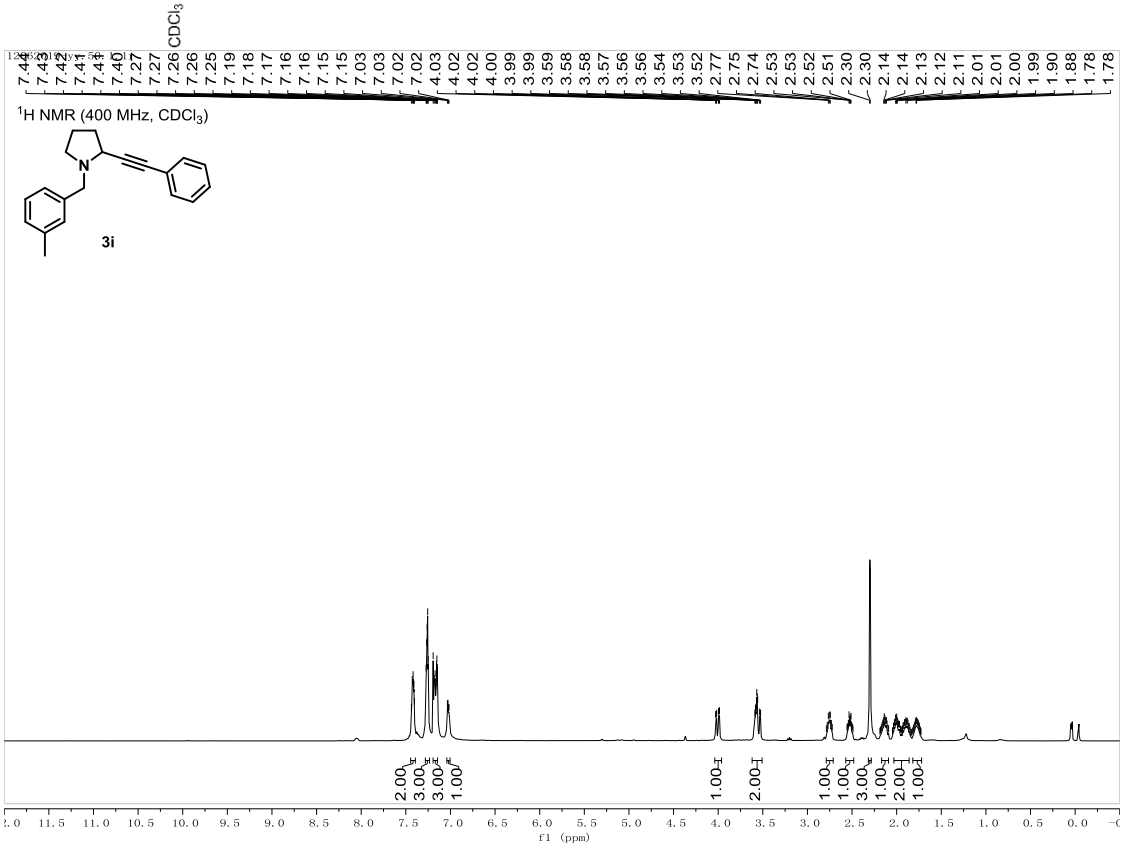

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
3f
f1 (ppm)

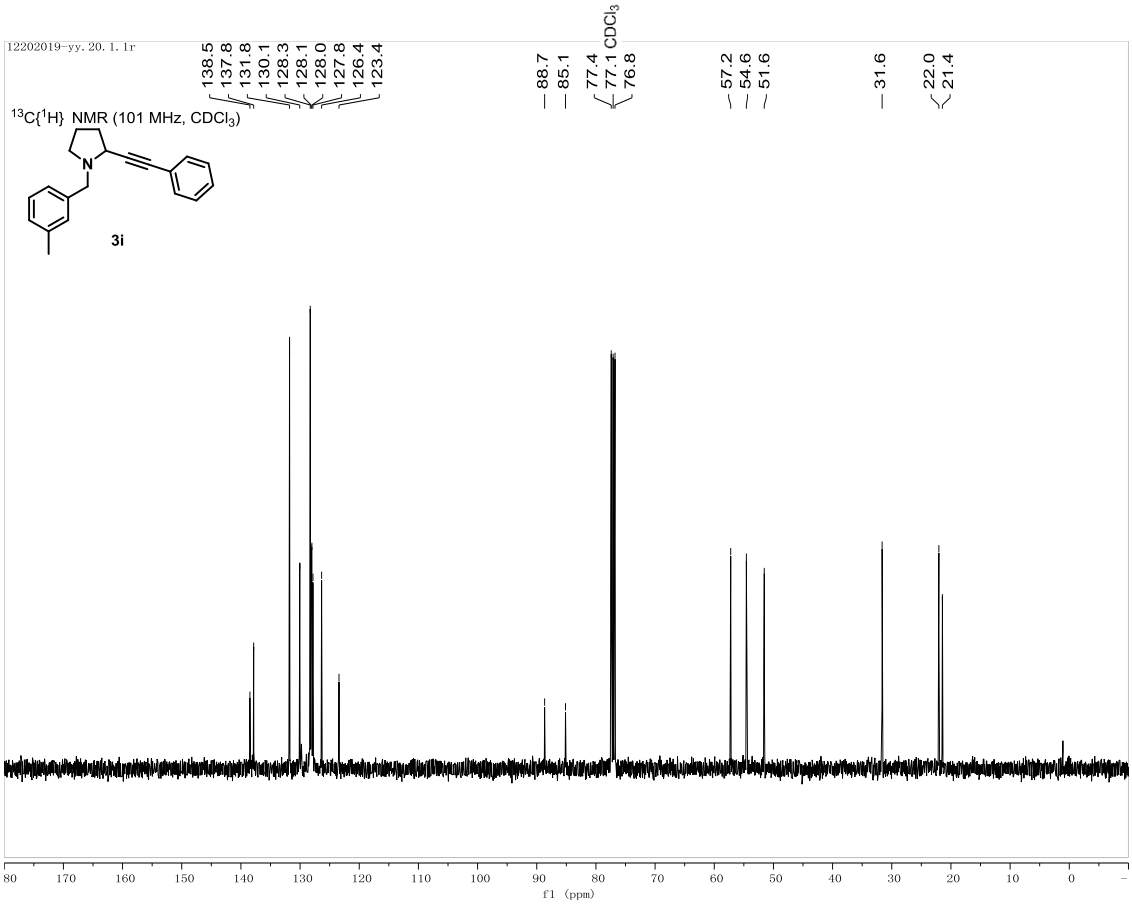

^{1}H NMR (400 MHz, CDCl$_3$)
3g

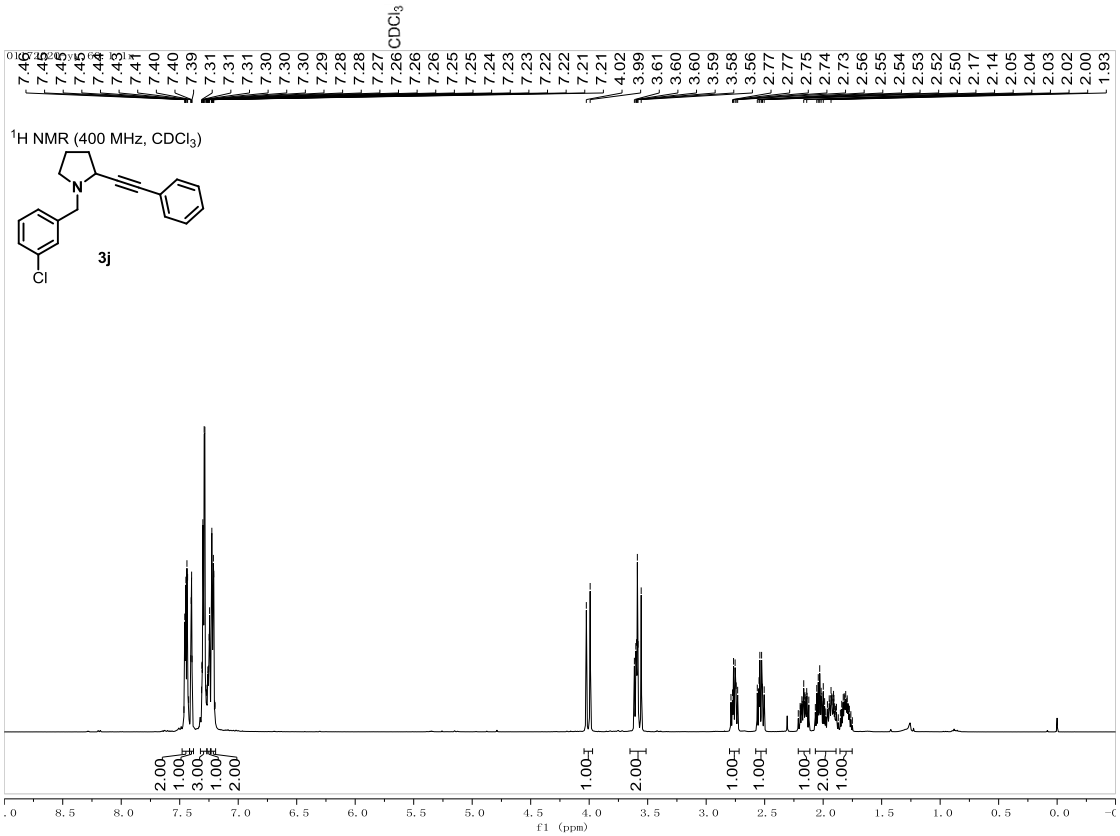

^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)
3g

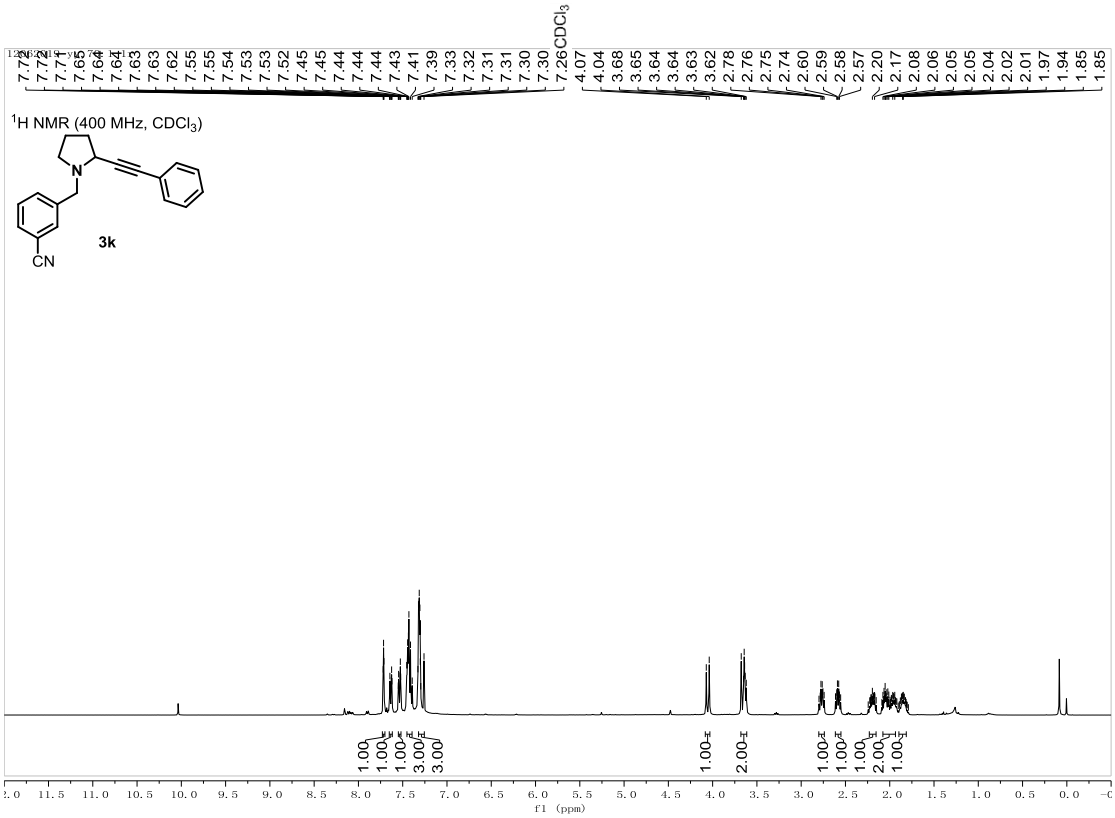

^{1}H NMR (400 MHz, $CDCl_3$)
3h
$CDCl_3$
f1 (ppm)

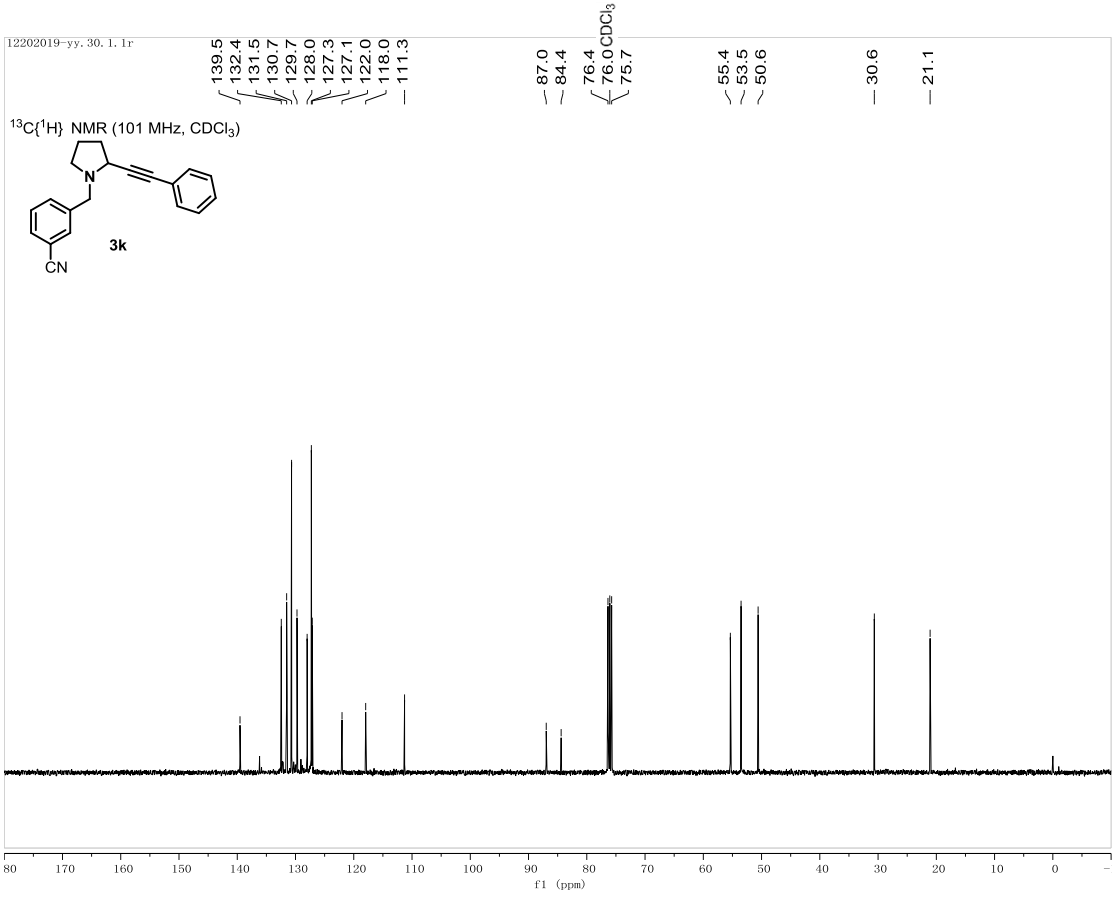

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
3h
$CDCl_3$
f1 (ppm)

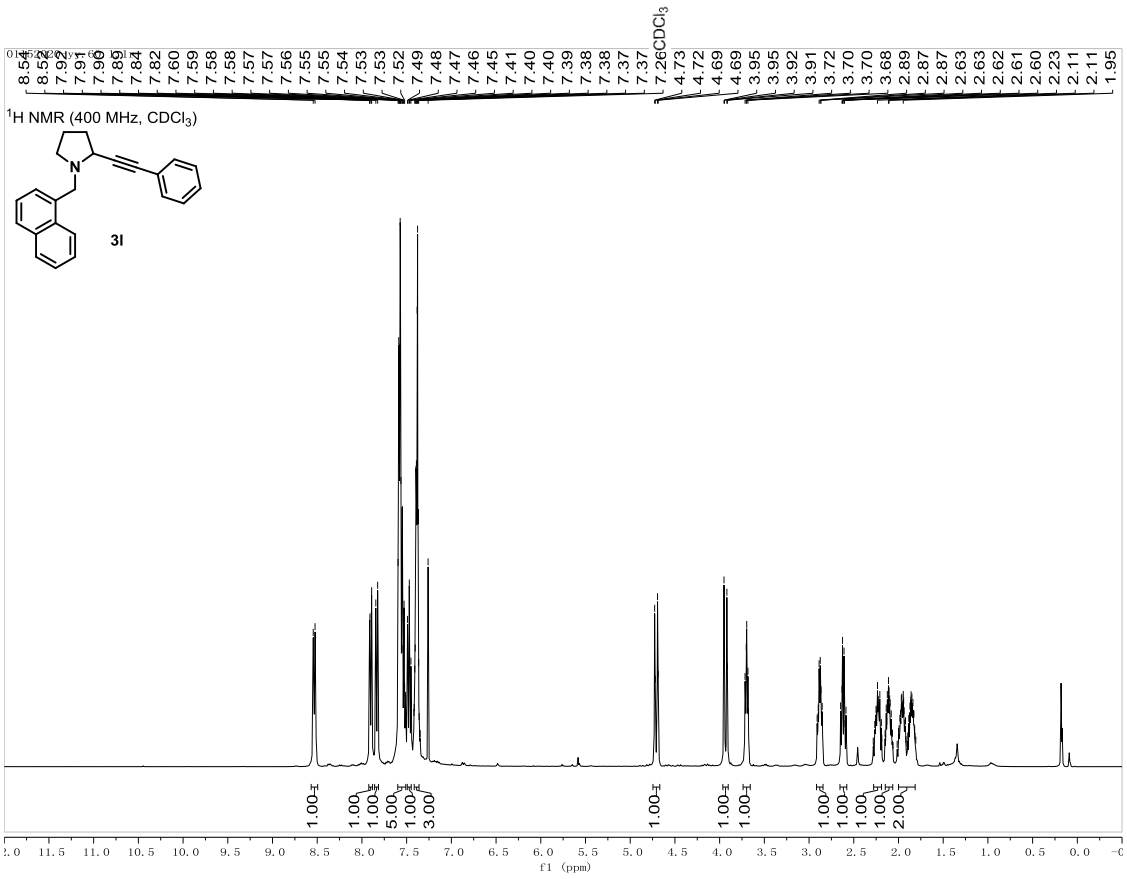

^{1}H NMR (400 MHz, $CDCl_3$)
3i
f1 (ppm)

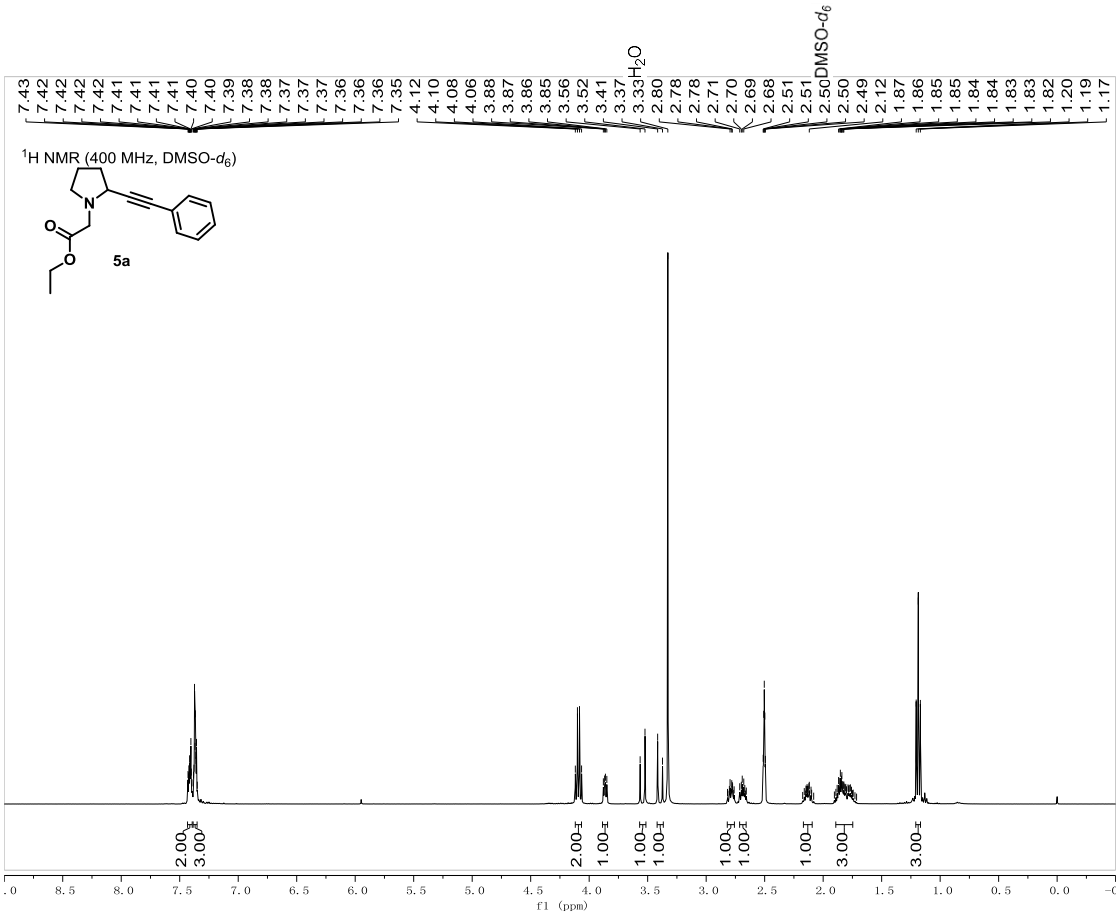

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
3i
f1 (ppm)

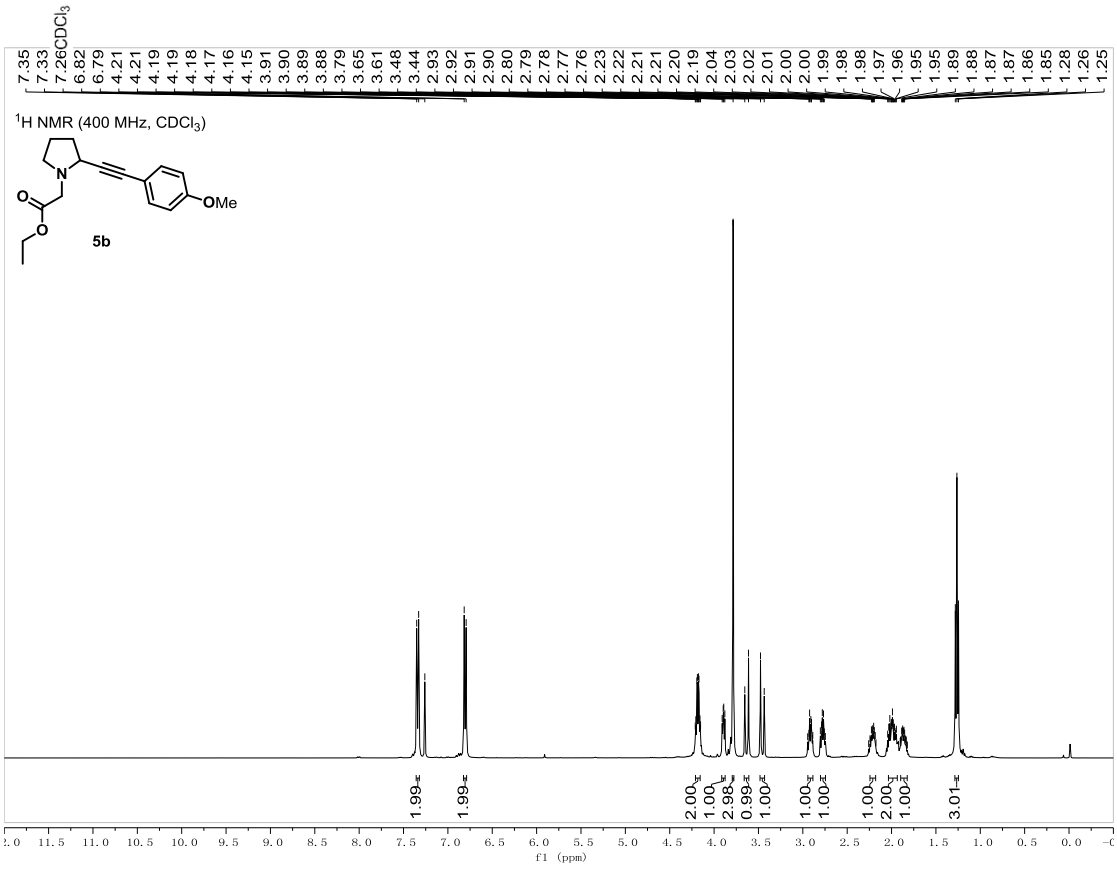

^{1}H NMR (400 MHz, $CDCl_3$)
3j
Cl
$CDCl_3$
f1 (ppm)

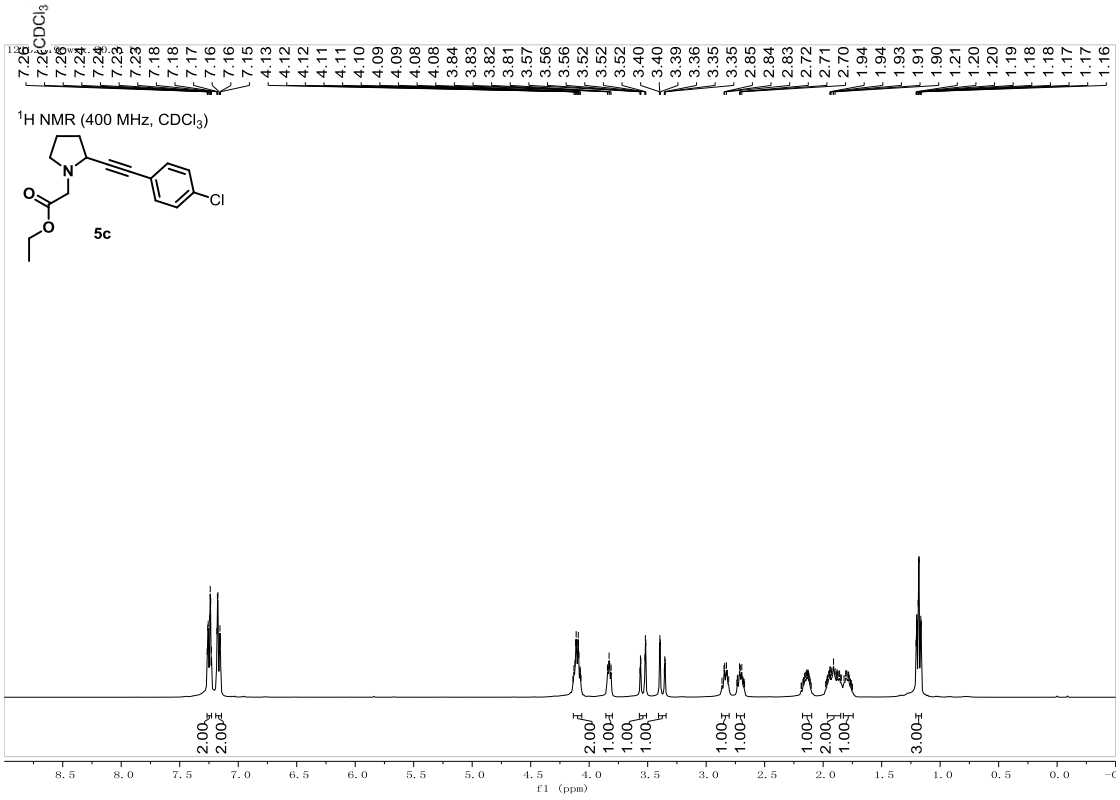

^{1}H NMR (400 MHz, $CDCl_3$)
3k
CN
7.26 $CDCl_3$
f1 (ppm)

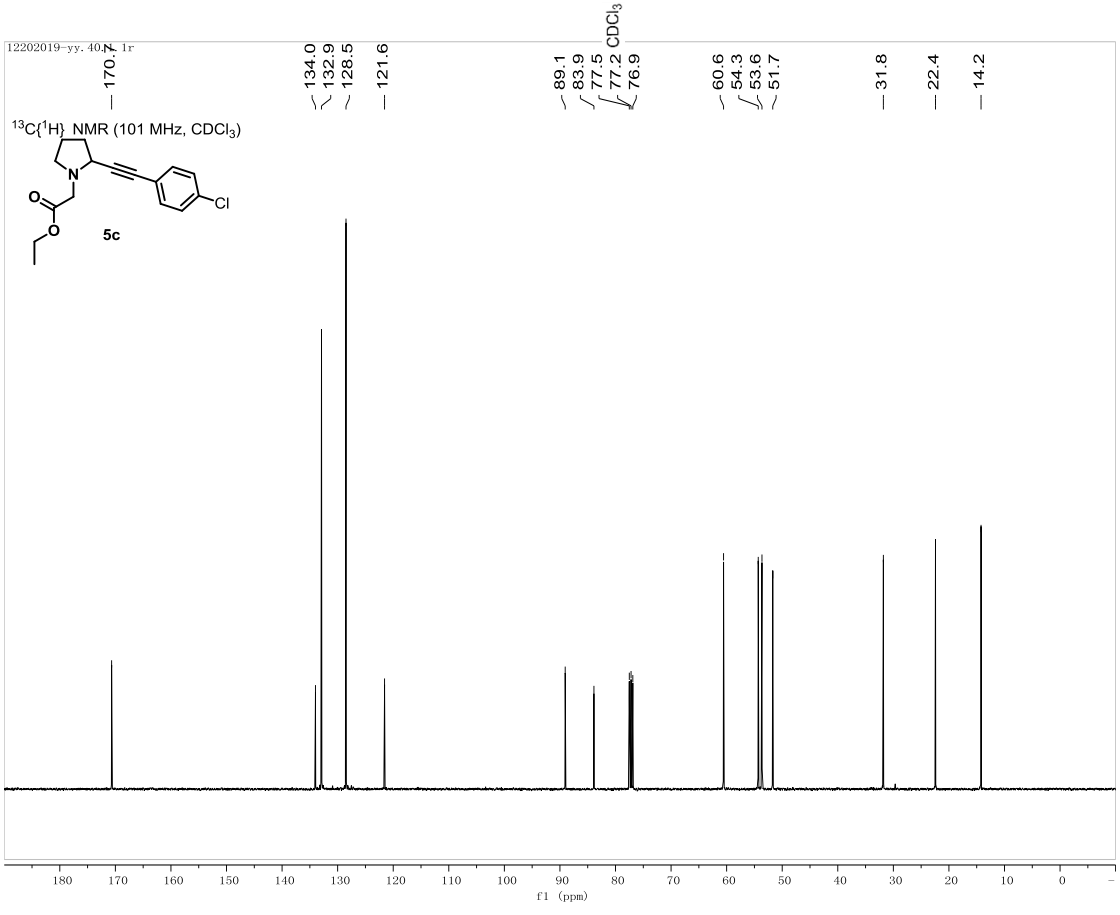

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
3k
CN
76.0 $CDCl_3$
f1 (ppm)

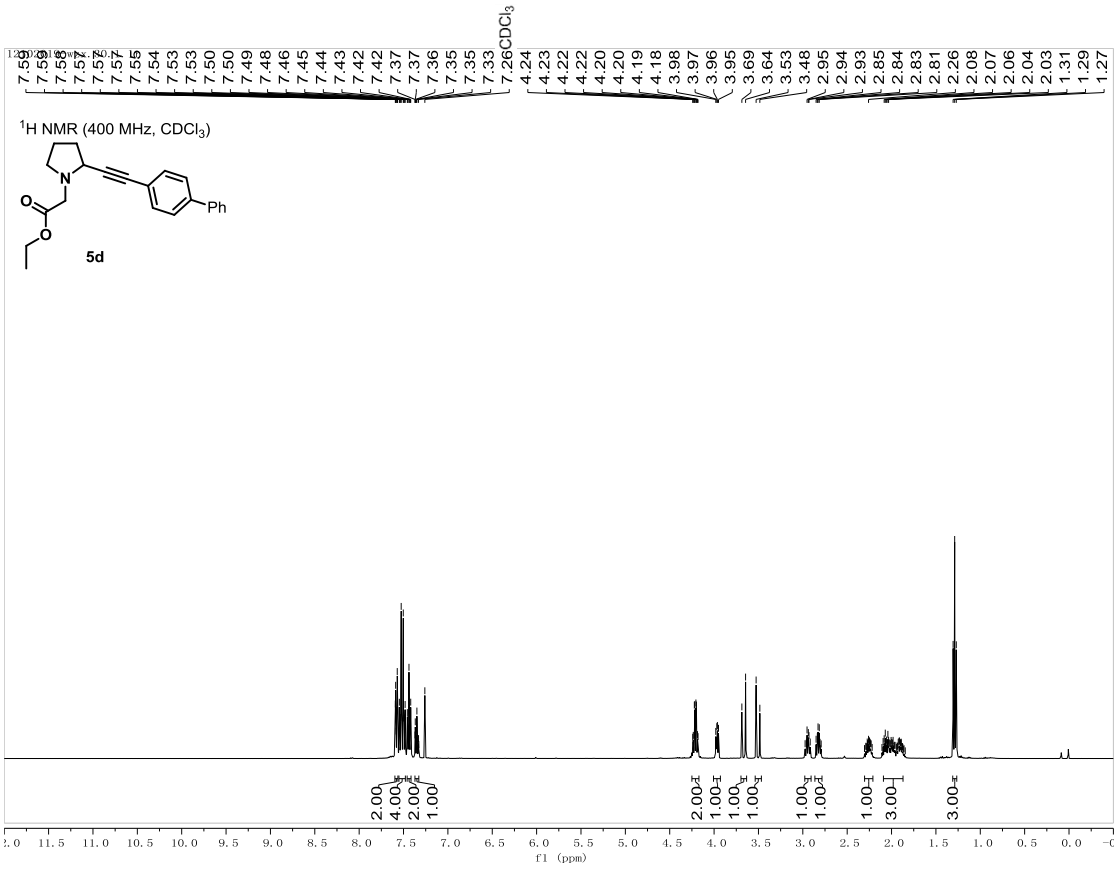

^{1}H NMR (400 MHz, $CDCl_3$)
3l
f1 (ppm)

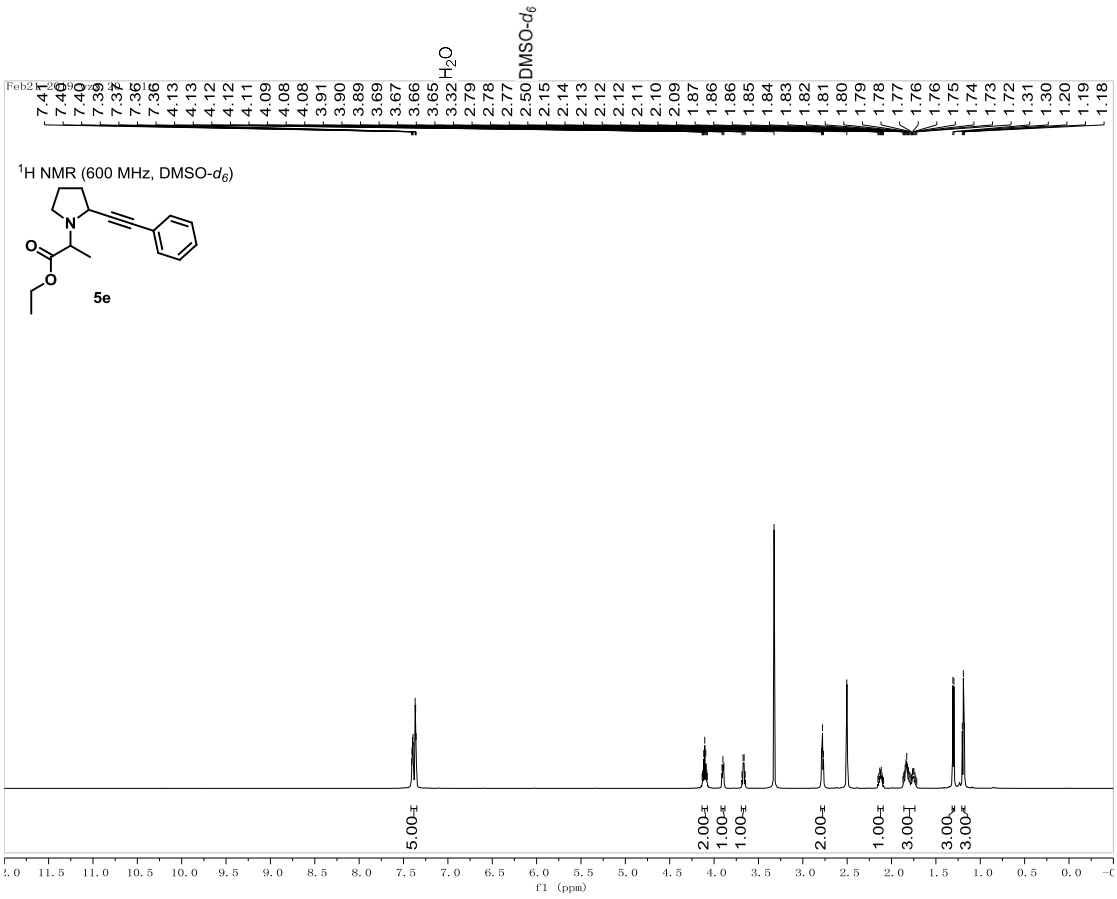

^{1}H NMR (400 MHz, DMSO-d_6)
5a
H$_2$O
DMSO-d_6
f1 (ppm)

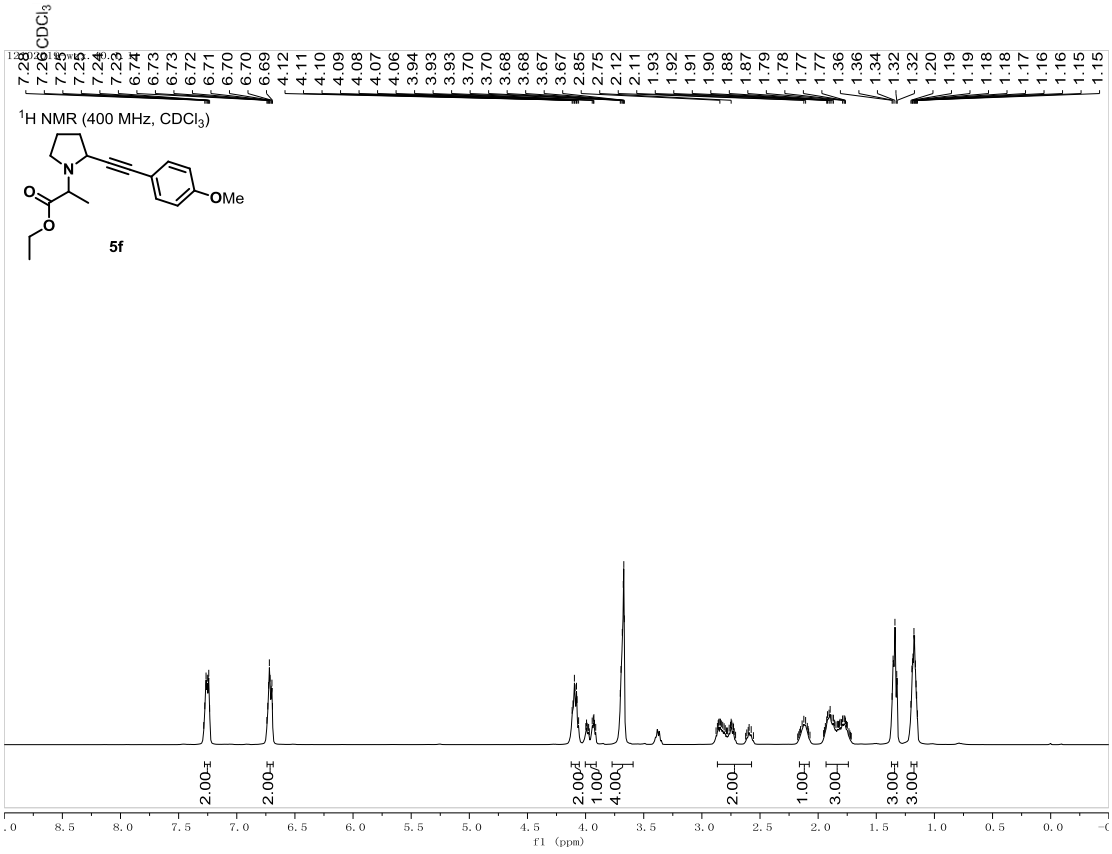

7.35
7.33
7.26CDCl3
6.82
6.79
4.21
4.21
4.19
4.19
4.18
4.17
4.16
4.15
3.91
3.90
3.89
3.88
3.79
3.65
3.61
3.48
3.44
2.93
2.92
2.91
2.90
2.80
2.79
2.78
2.77
2.76
2.23
2.22
2.21
2.21
2.20
2.19
2.04
2.03
2.02
2.01
2.00
2.00
1.99
1.98
1.98
1.97
1.96
1.95
1.95
1.89
1.88
1.87
1.87
1.86
1.85
1.28
1.26
1.25
1H NMR (400 MHz, CDCl3)
N
O
O
OMe
5b
1.99
1.99
2.00
1.00
2.98
0.99
1.00
1.00
1.00
1.00
2.00
1.00
3.01
f1 (ppm)

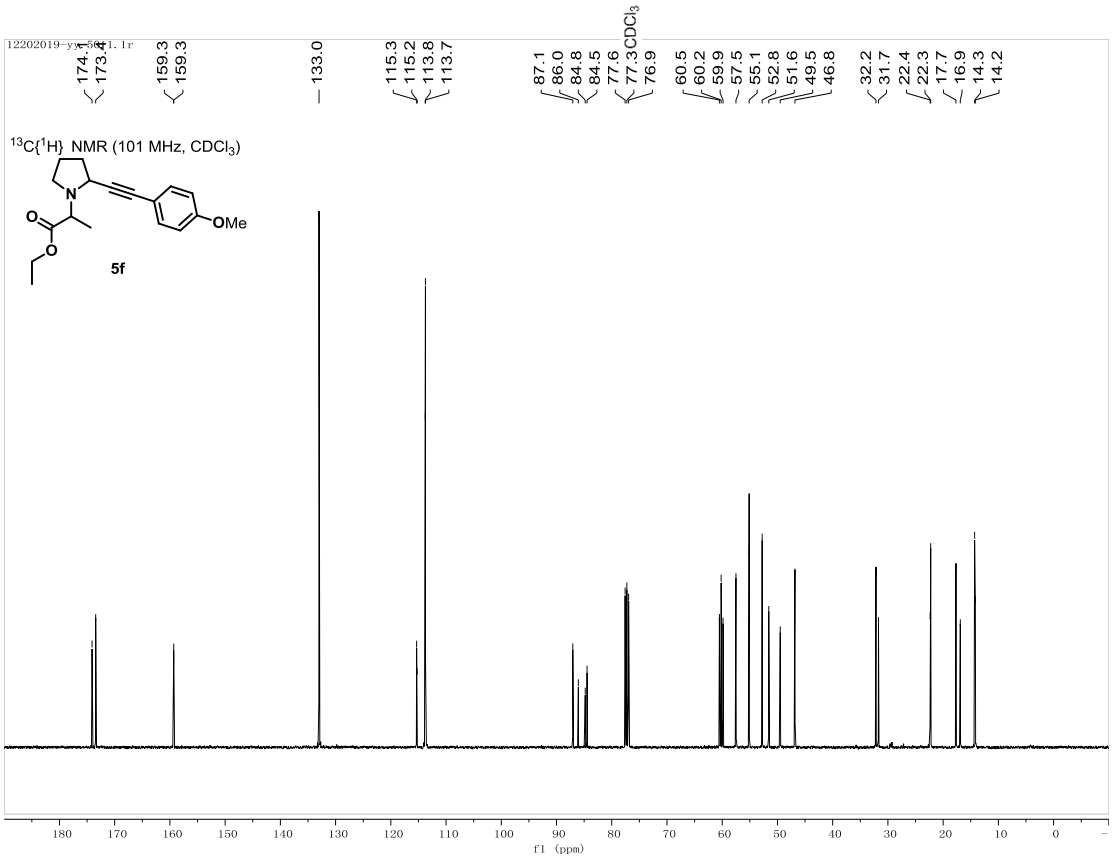

^{1}H NMR (400 MHz, $CDCl_3$)
5c
Cl
f1 (ppm)

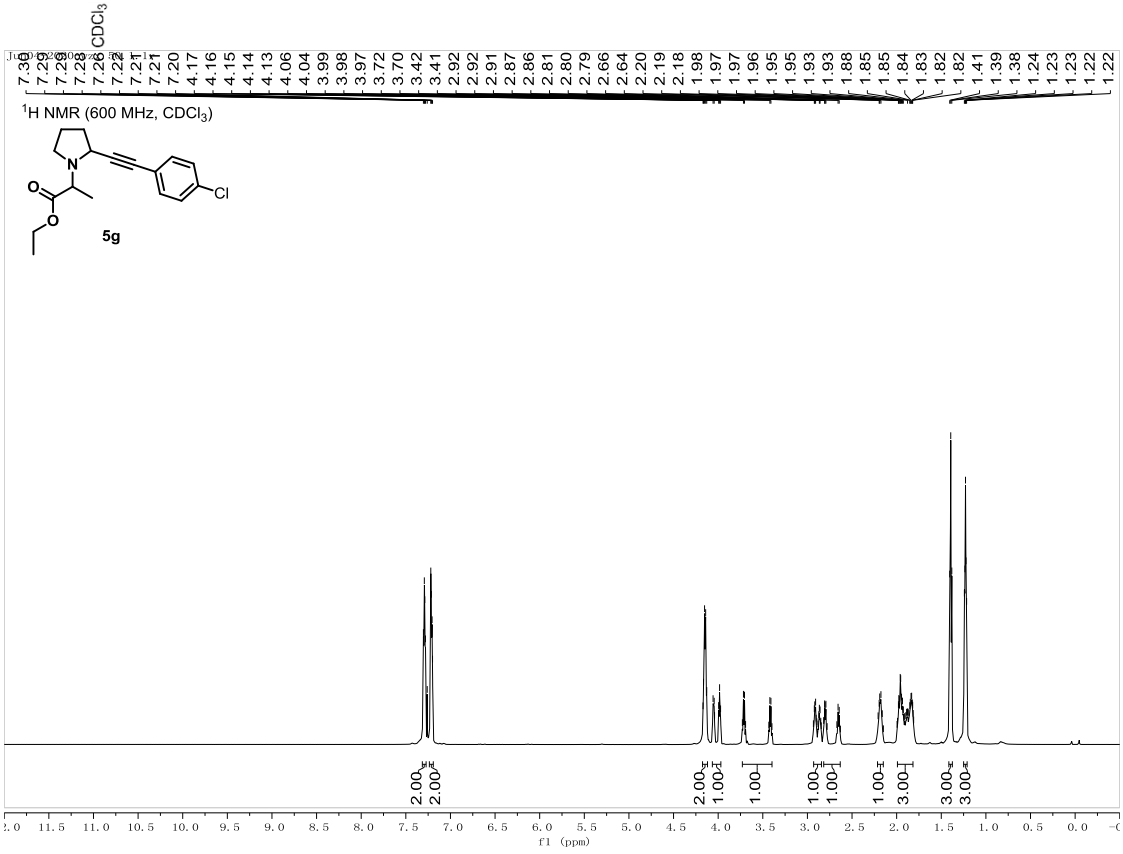

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
5c
Cl
CDCl3
f1 (ppm)

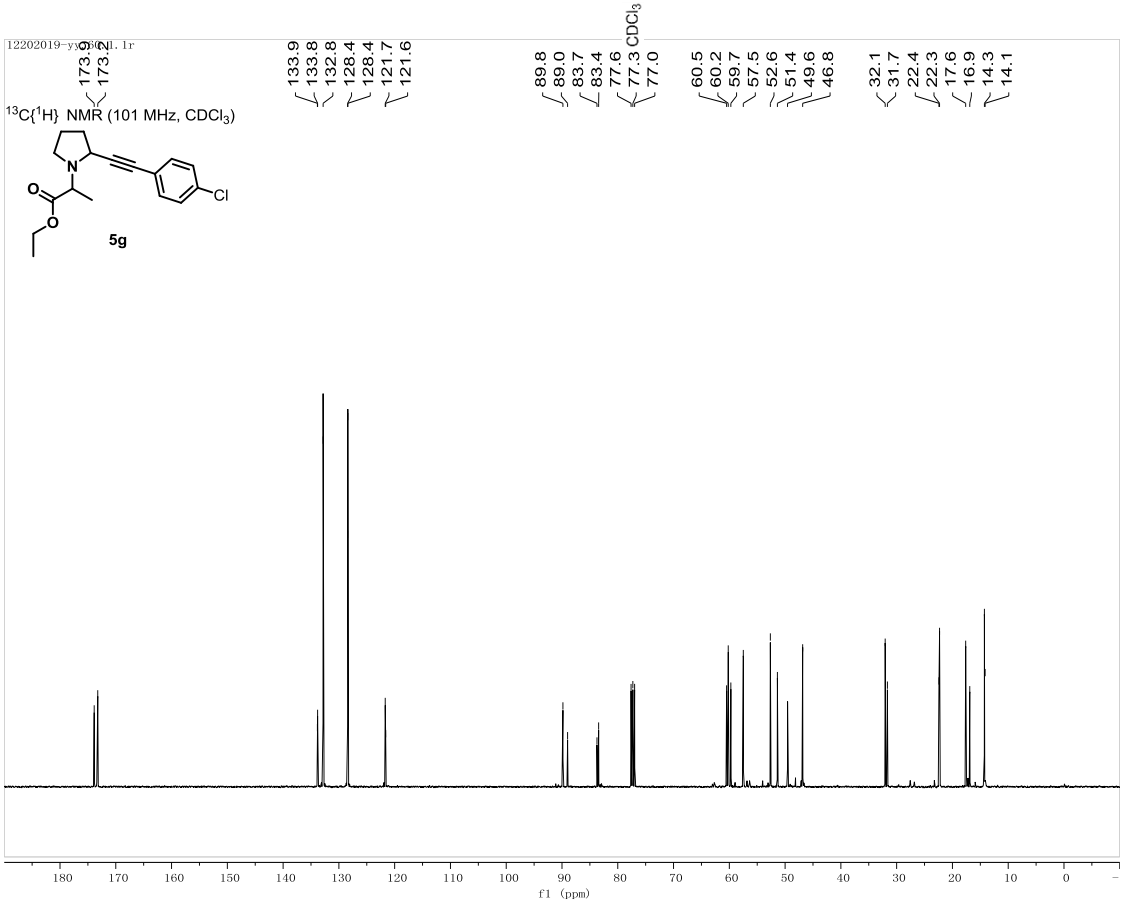

^{1}H NMR (400 MHz, $CDCl_3$)
Ph
5d
f1 (ppm)

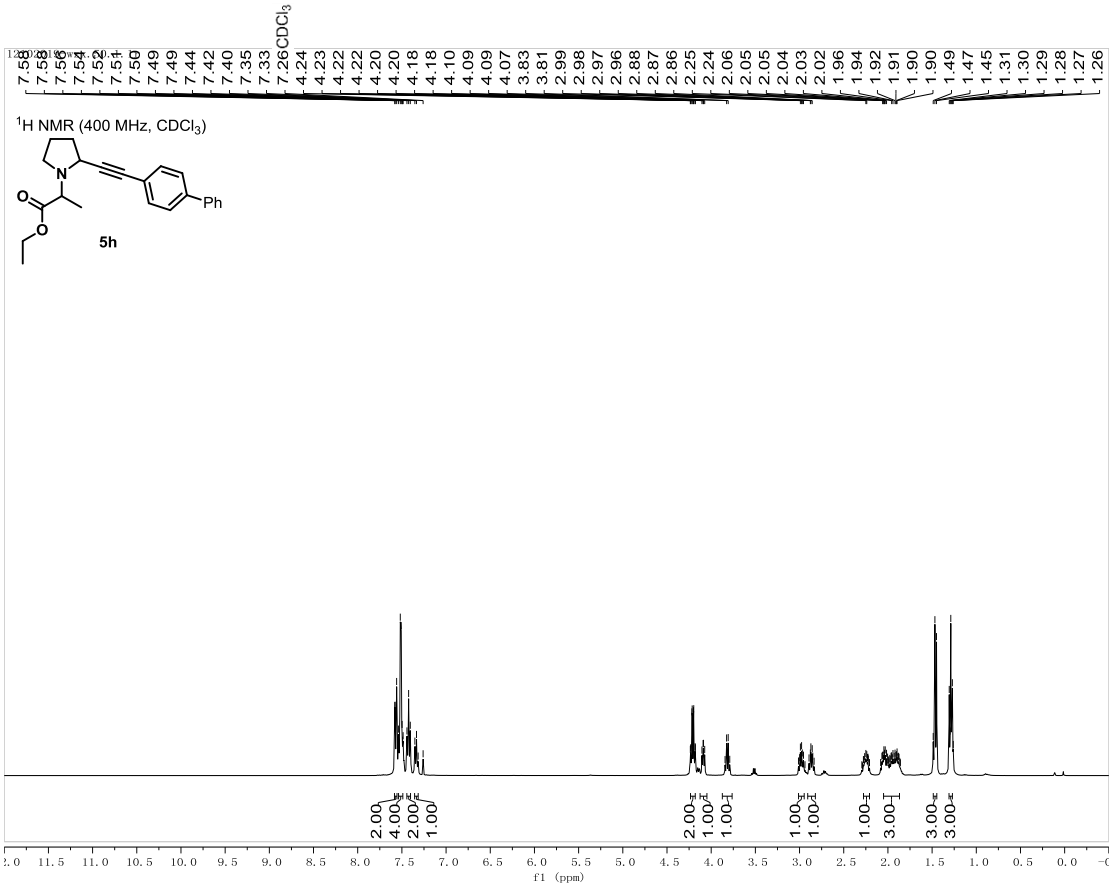

H2O
DMSO-d6
1H NMR (600 MHz, DMSO-d6)
5e
5.00
2.00
1.00
1.00
2.00
1.00
3.00
3.00
f1 (ppm)

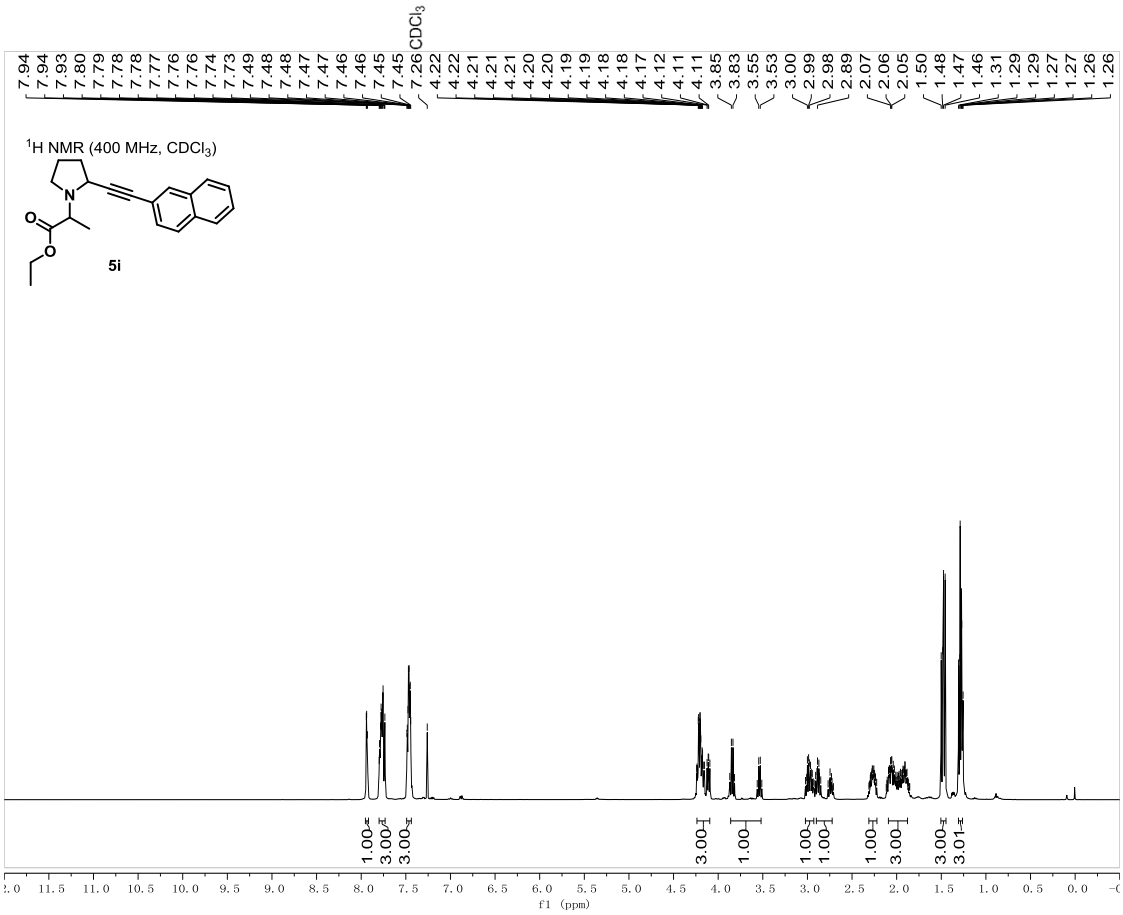

^{1}H NMR (400 MHz, $CDCl_3$)
OMe
5f

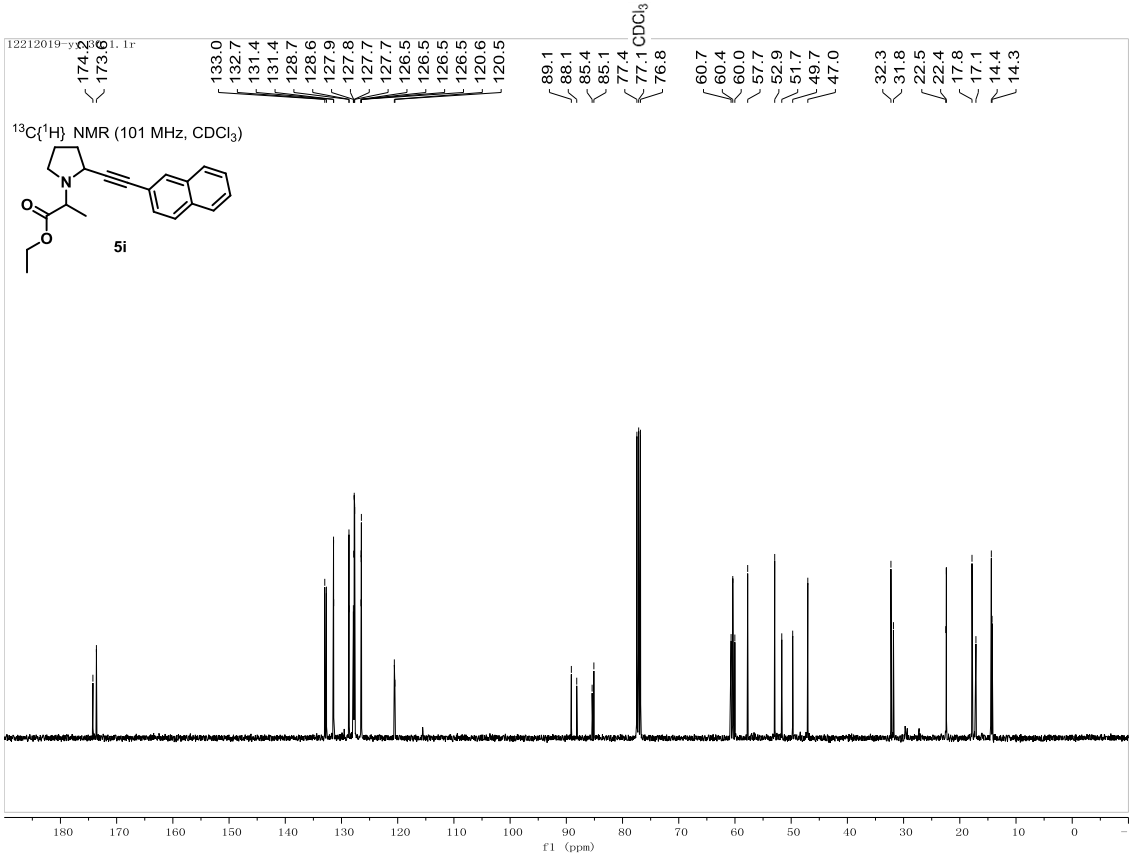

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
OMe
5f


^{1}H NMR (600 MHz, $CDCl_3$)
5g
Cl
$CDCl_3$
f1 (ppm)

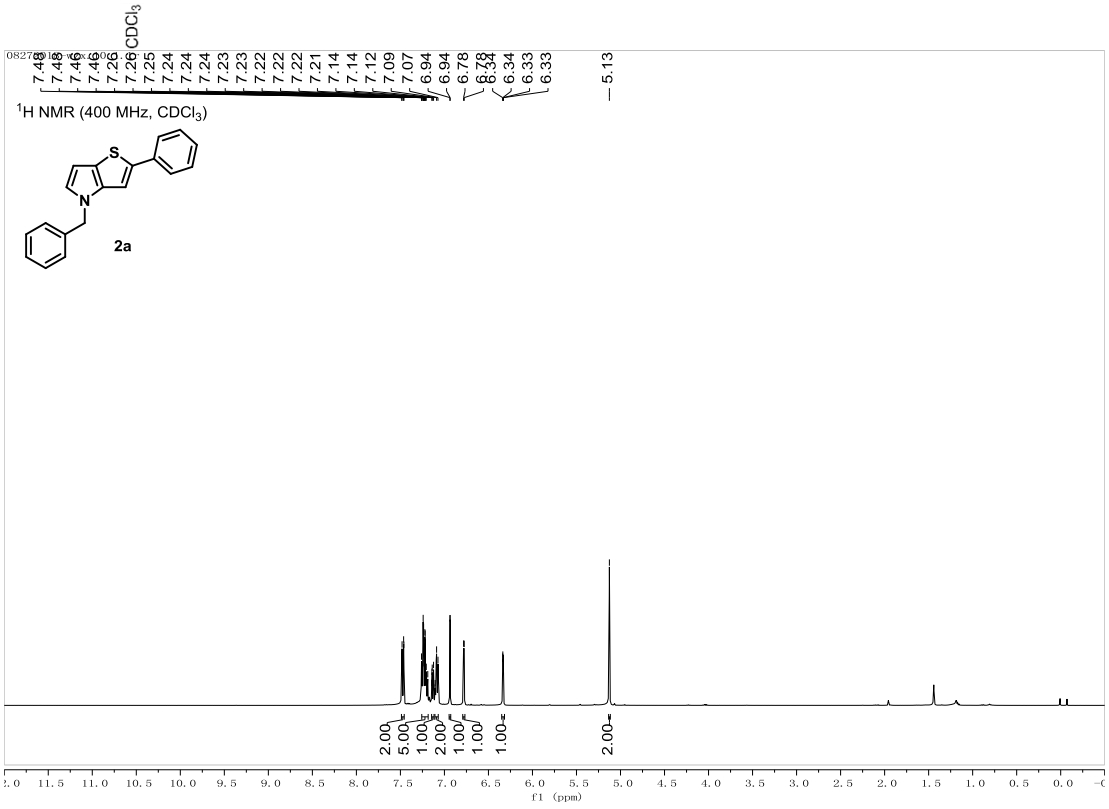

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
5g
Cl
$CDCl_3$
f1 (ppm)

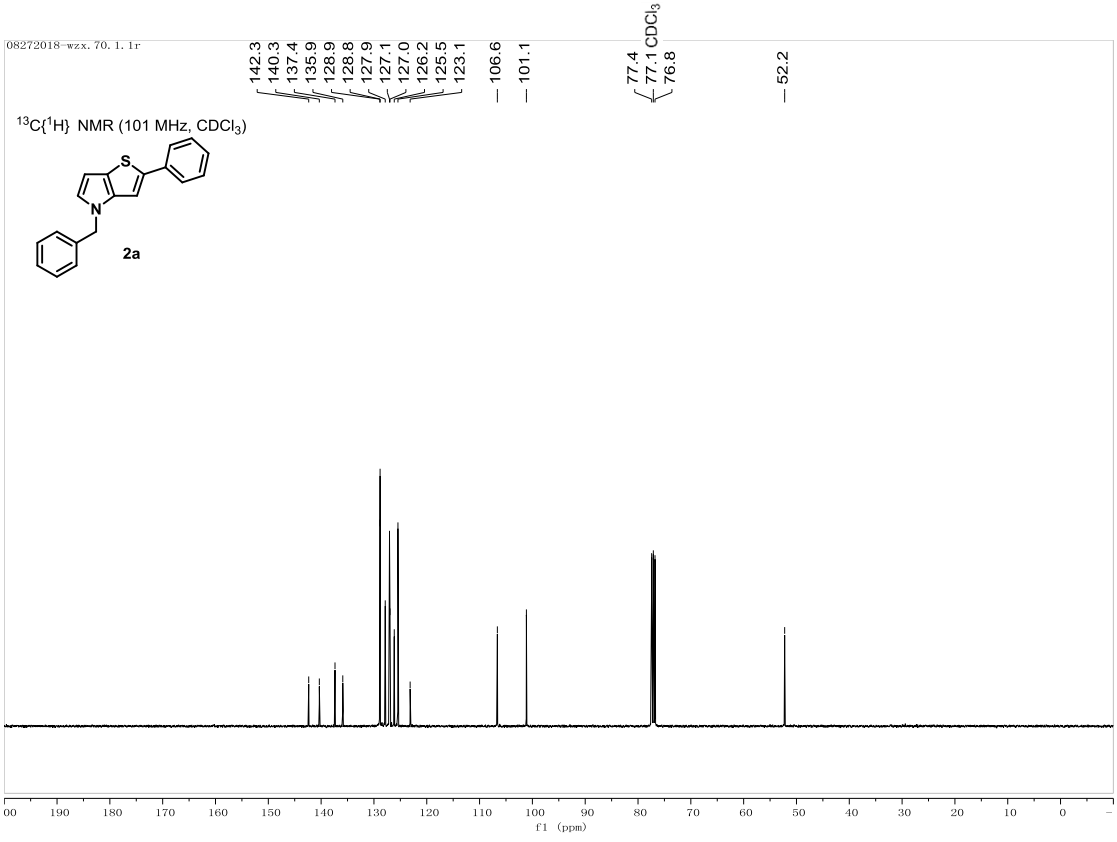

^{1}H NMR (400 MHz, $CDCl_3$)
5h
Ph
$CDCl_3$
f1 (ppm)

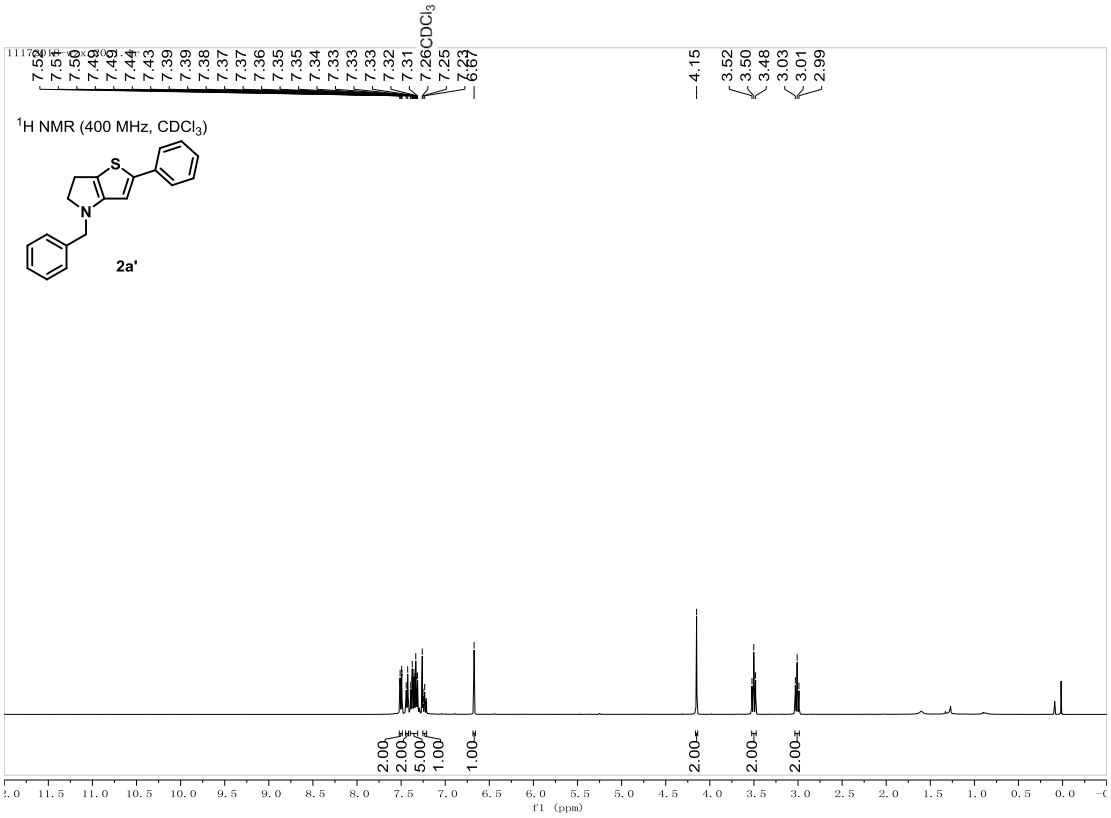

7.94 7.94 7.93 7.80 7.79 7.78 7.78 7.77 7.76 7.76 7.74 7.73 7.49 7.48 7.48 7.47 7.47 7.46 7.46 7.45 7.45 7.26 CDCl3 4.22 4.22 4.21 4.21 4.20 4.20 4.19 4.19 4.18 4.18 4.17 4.12 4.11 4.11 3.85 3.83 3.55 3.53 3.00 2.99 2.98 2.89 2.07 2.06 2.05 1.50 1.48 1.47 1.46 1.31 1.29 1.29 1.27 1.27 1.26 1.26
1H NMR (400 MHz, CDCl3)
5i
1.00 3.00 3.00 3.00 1.00 1.00 1.00 1.00 3.00 3.00 3.01
f1 (ppm)

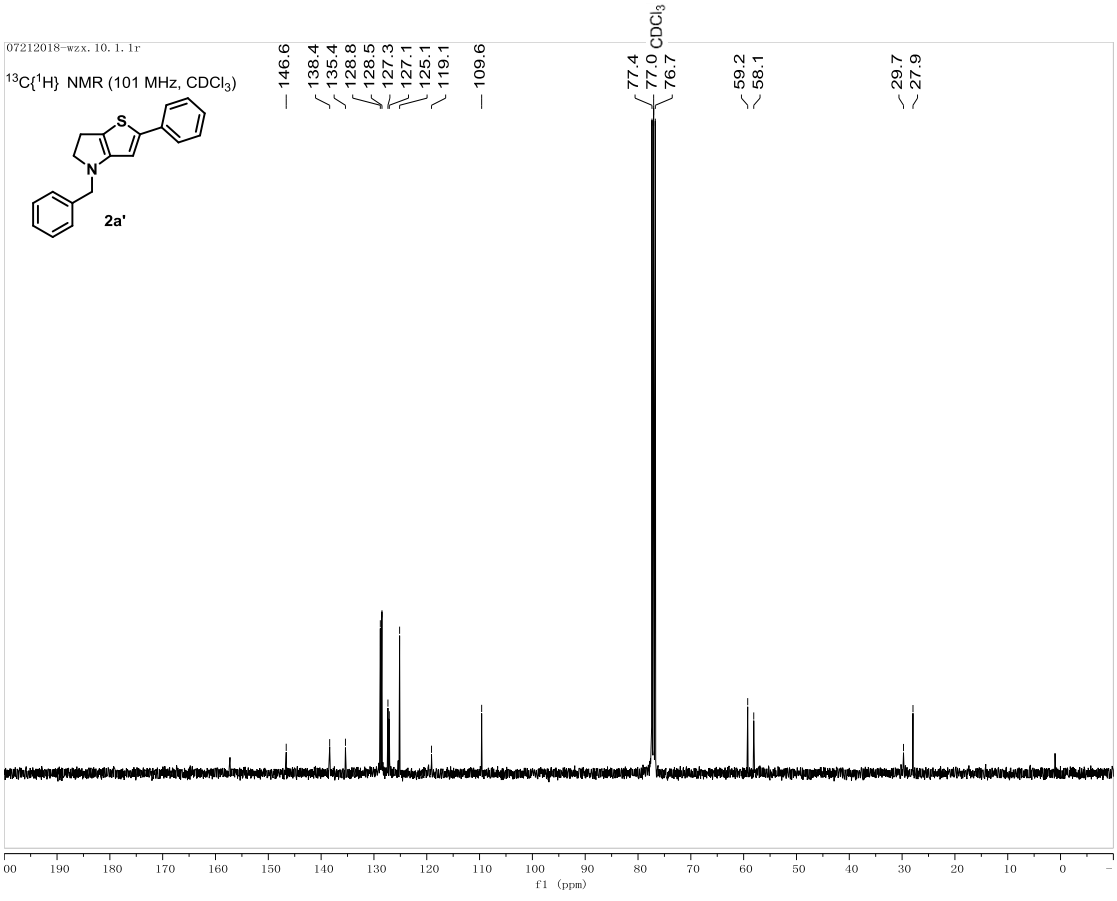

174.2 173.6 133.0 132.7 131.4 131.4 128.7 128.6 127.9 127.8 127.7 127.7 126.5 126.5 126.5 126.5 120.6 120.5 89.1 88.1 85.4 85.1 77.4 77.1 CDCl3 76.8 60.7 60.4 60.0 57.7 52.9 51.7 49.7 47.0 32.3 31.8 22.5 22.4 17.8 17.1 14.4 14.3
13C{1H} NMR (101 MHz, CDCl3)
5i
f1 (ppm)

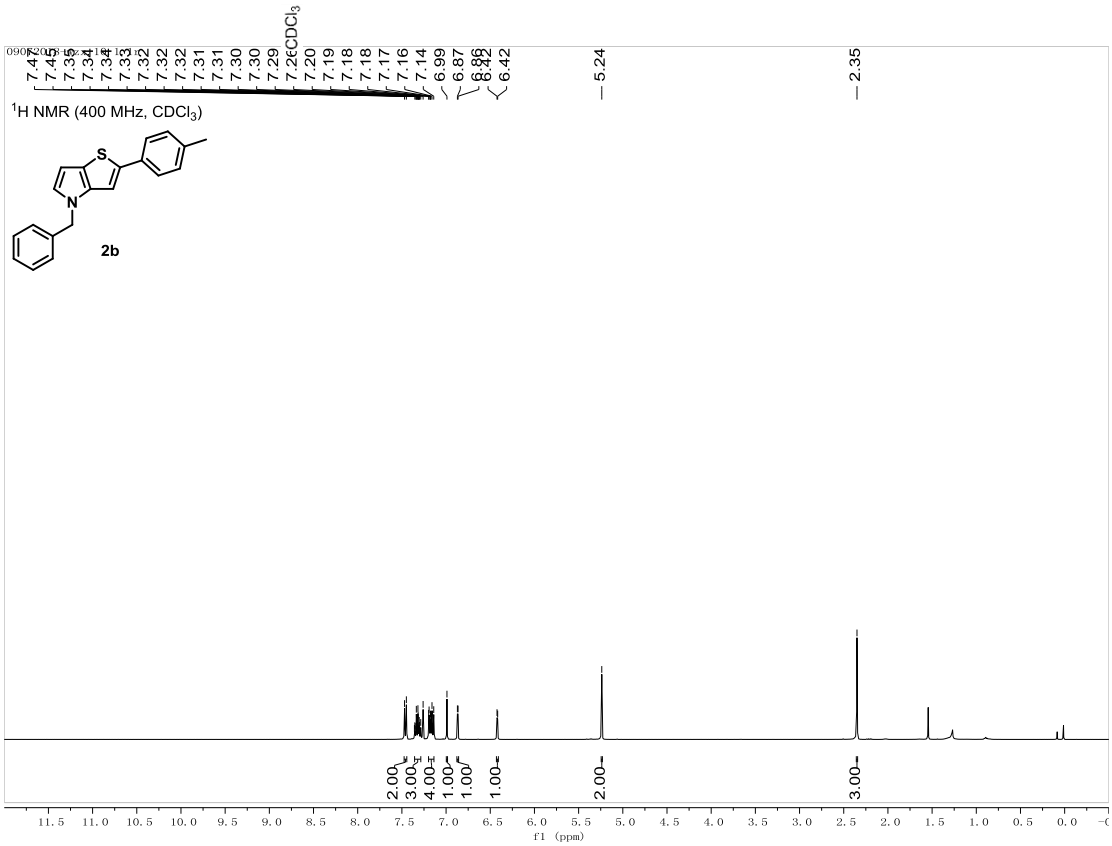
4. ^{1}H NMR and ^{13}C {^{1}H} NMR copies of products

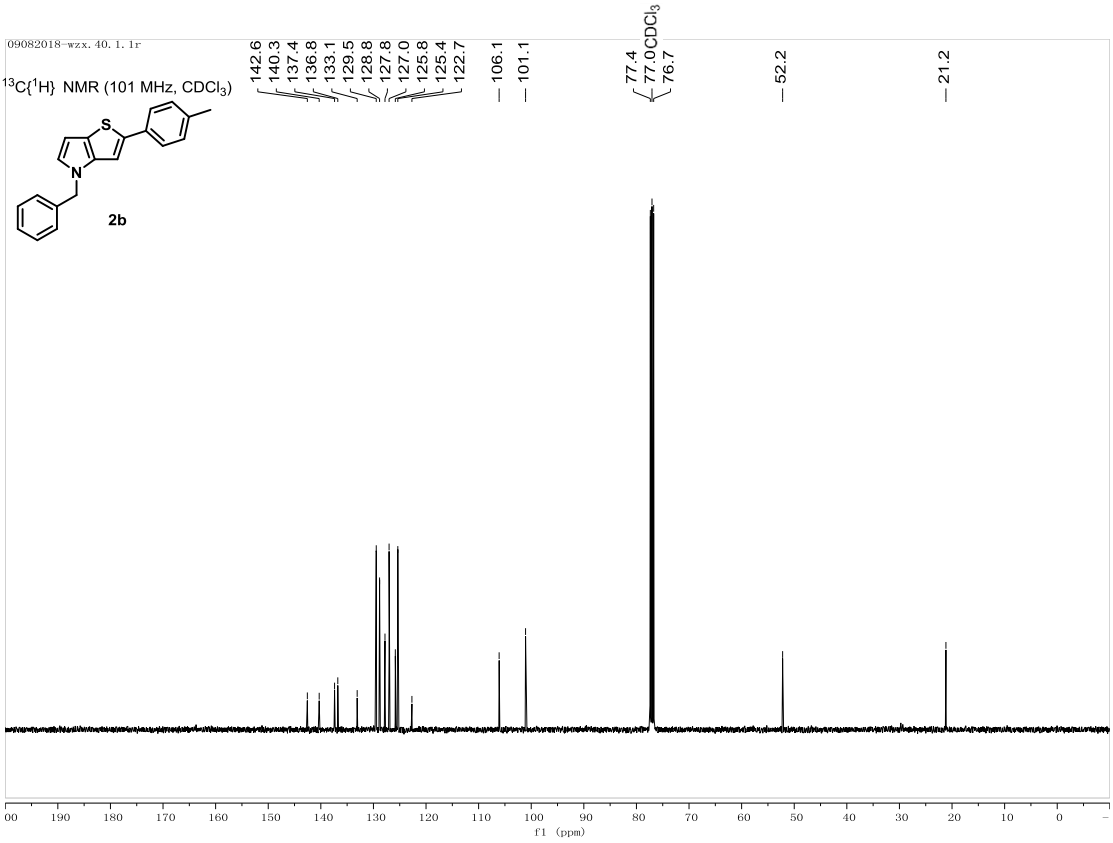


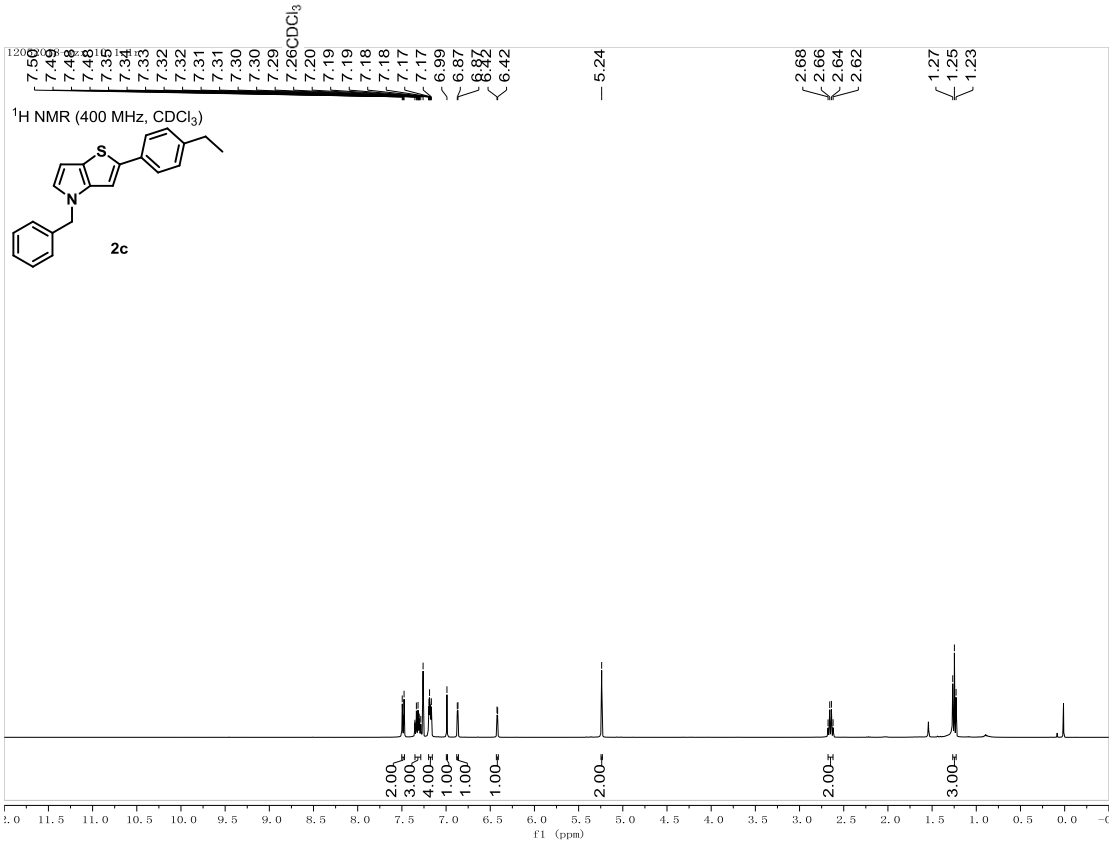


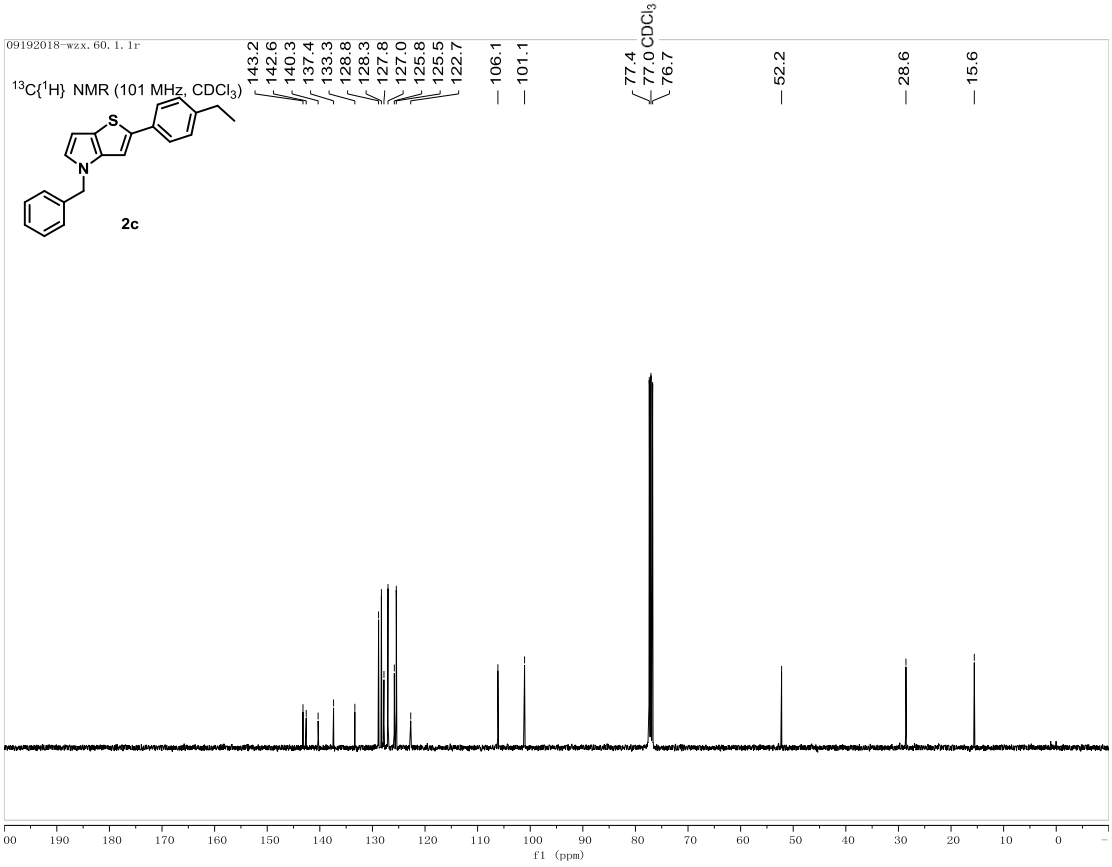

7.52
7.51
7.50
7.49
7.44
7.43
7.39
7.39
7.38
7.37
7.37
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.31
7.26CDCl3
7.25
7.23
6.67
4.15
3.52
3.50
3.48
3.03
3.01
2.99
1H NMR (400 MHz, CDCl3)
S
N
2a'
2.00
2.00
5.00
1.00
1.00
2.00
2.00
2.00
f1 (ppm)

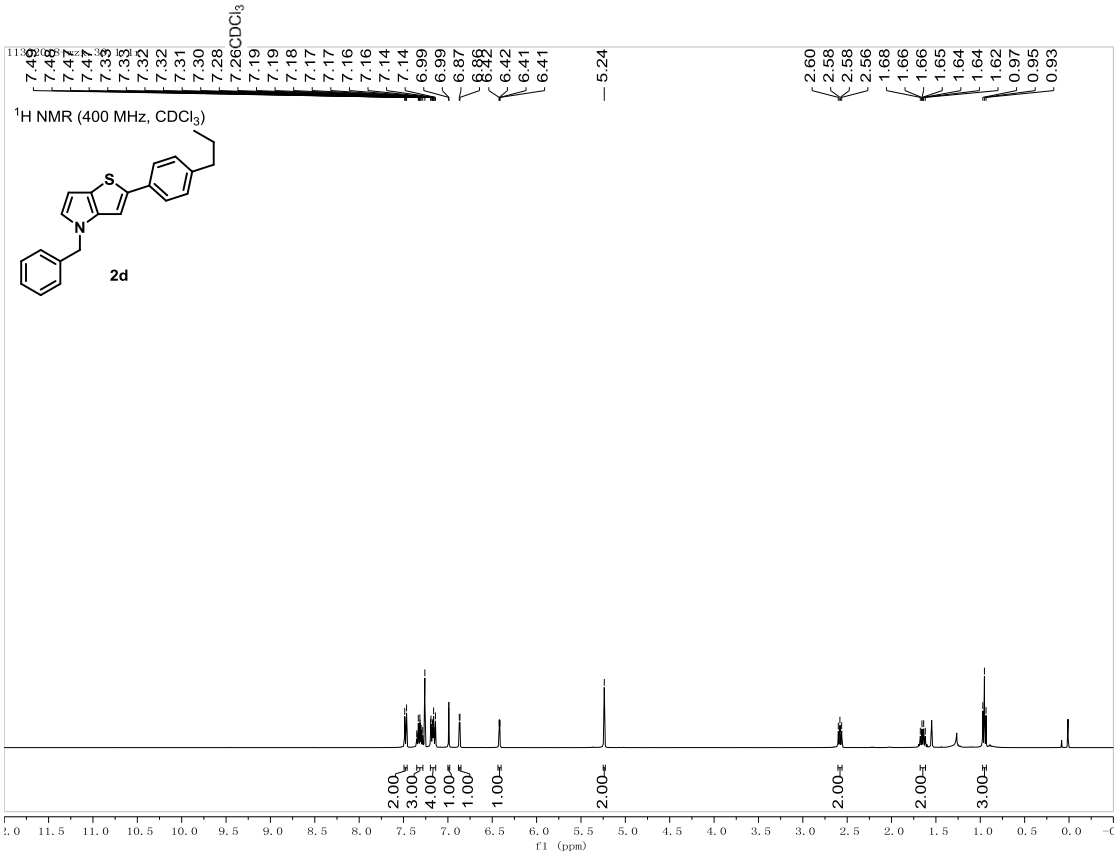

07212018-wzx. 10. 1. 1r
13C{1H} NMR (101 MHz, CDCl3)
146.6
138.4
135.4
128.8
128.5
127.3
127.1
125.1
119.1
109.6
77.4
77.0 CDCl3
76.7
59.2
58.1
29.7
27.9
S
N
2a'
f1 (ppm)

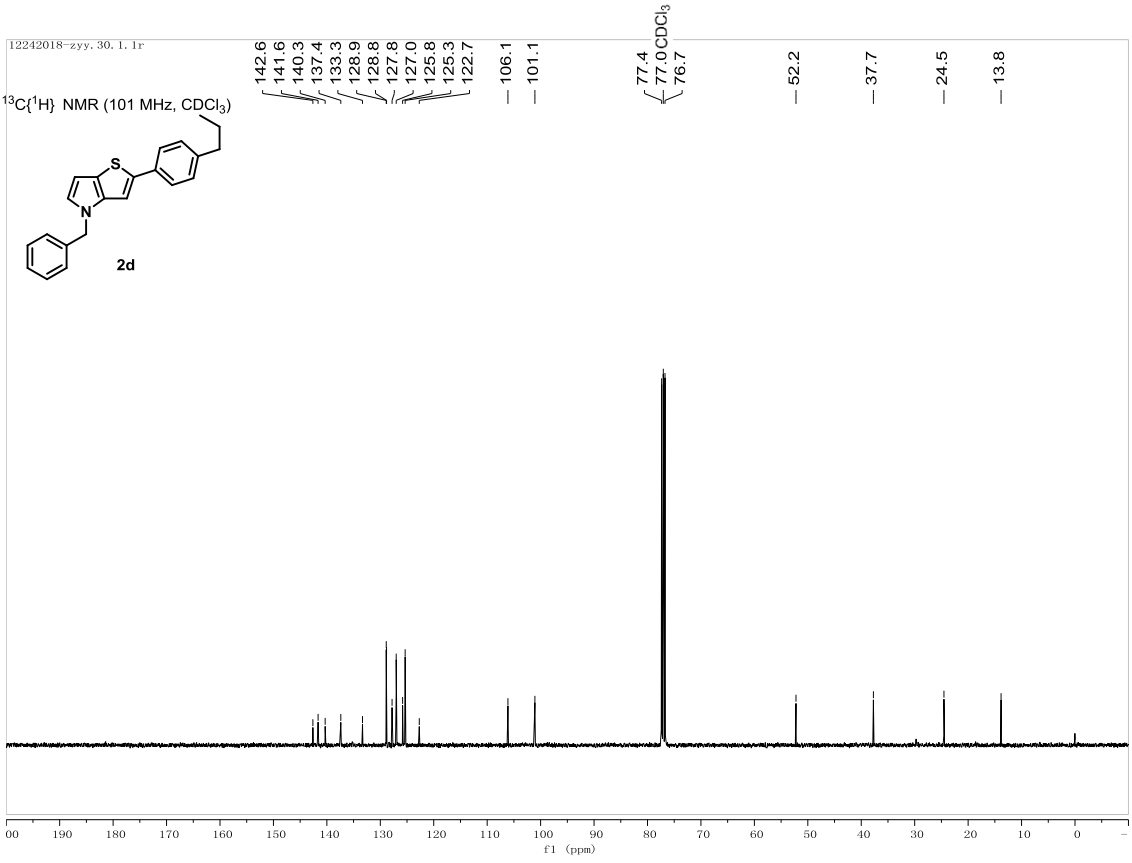

^{1}H NMR (400 MHz, $CDCl_3$)
2b

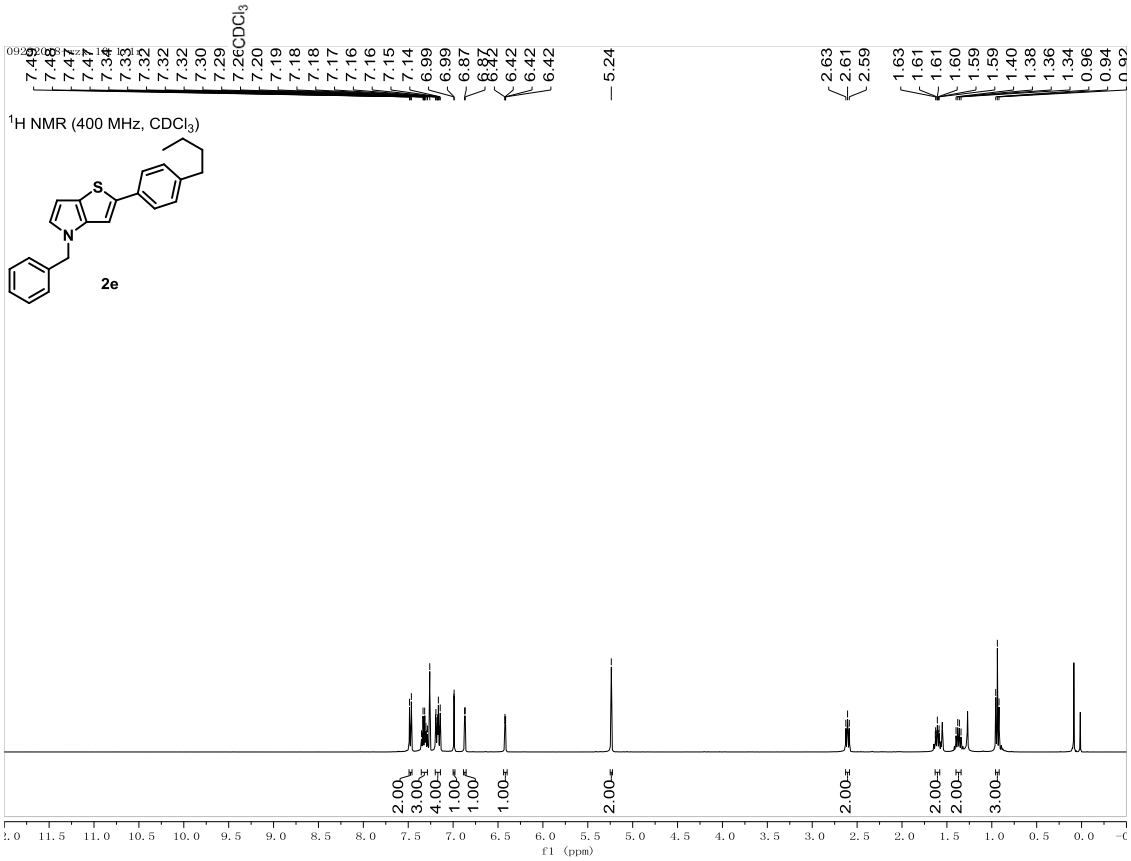

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
2b

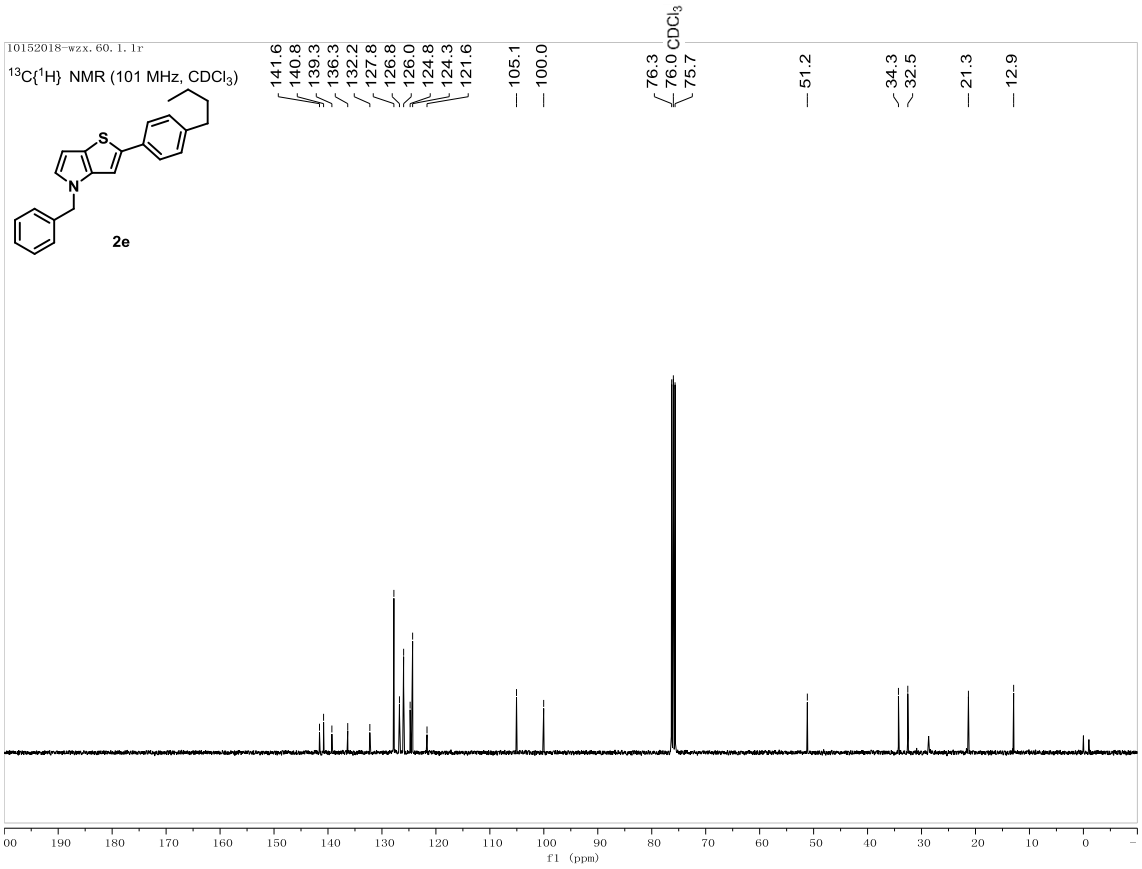

7.50
7.49
7.48
7.48
7.35
7.34
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.29
7.26CDCl3
7.20
7.19
7.19
7.18
7.18
7.17
7.17
6.99
6.87
6.87
6.42
6.42
5.24
2.68
2.66
2.64
2.62
1.27
1.25
1.23
1H NMR (400 MHz, CDCl3)
2c
2.00
3.00
4.00
1.00
1.00
1.00
2.00
2.00
3.00
f1 (ppm)

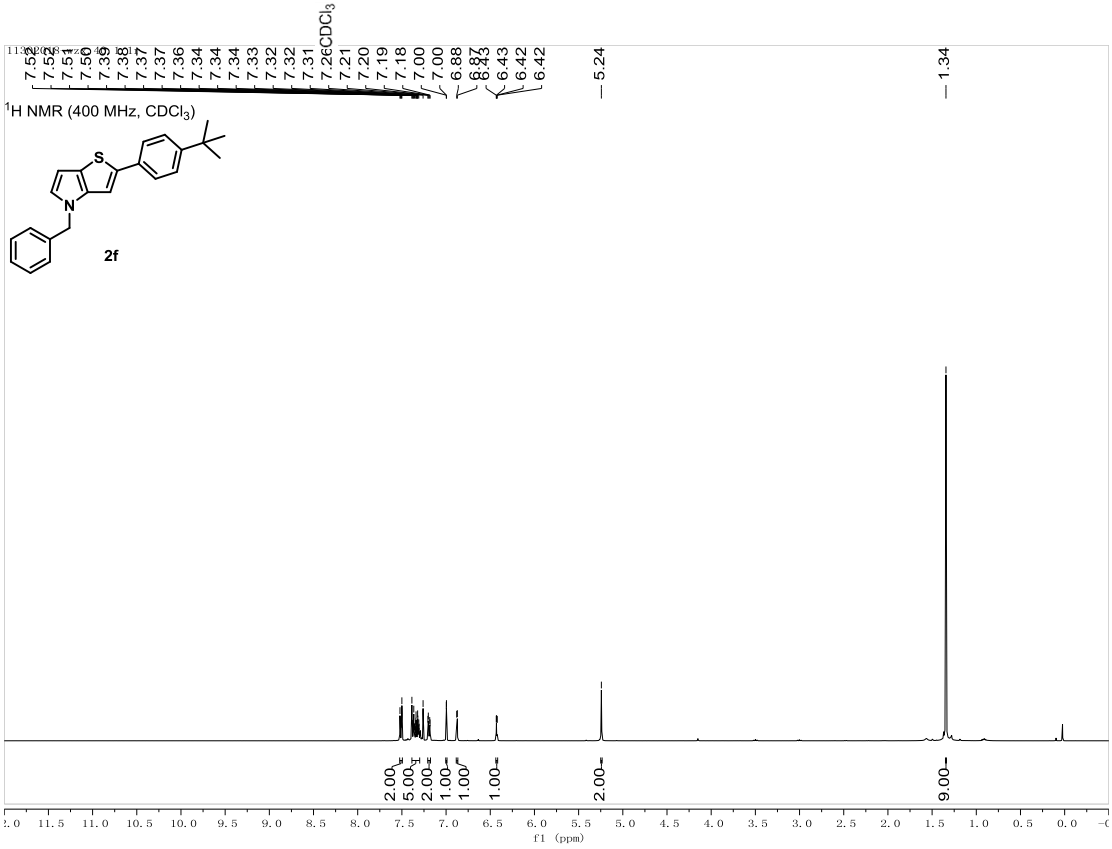

09192018-wzx. 60. 1. 1r
143.2
142.6
140.3
137.4
133.3
128.8
128.3
127.8
127.0
125.8
125.5
122.7
106.1
101.1
77.4
77.0CDCl3
76.7
52.2
28.6
15.6
13C{1H} NMR (101 MHz, CDCl3)
2c
f1 (ppm)

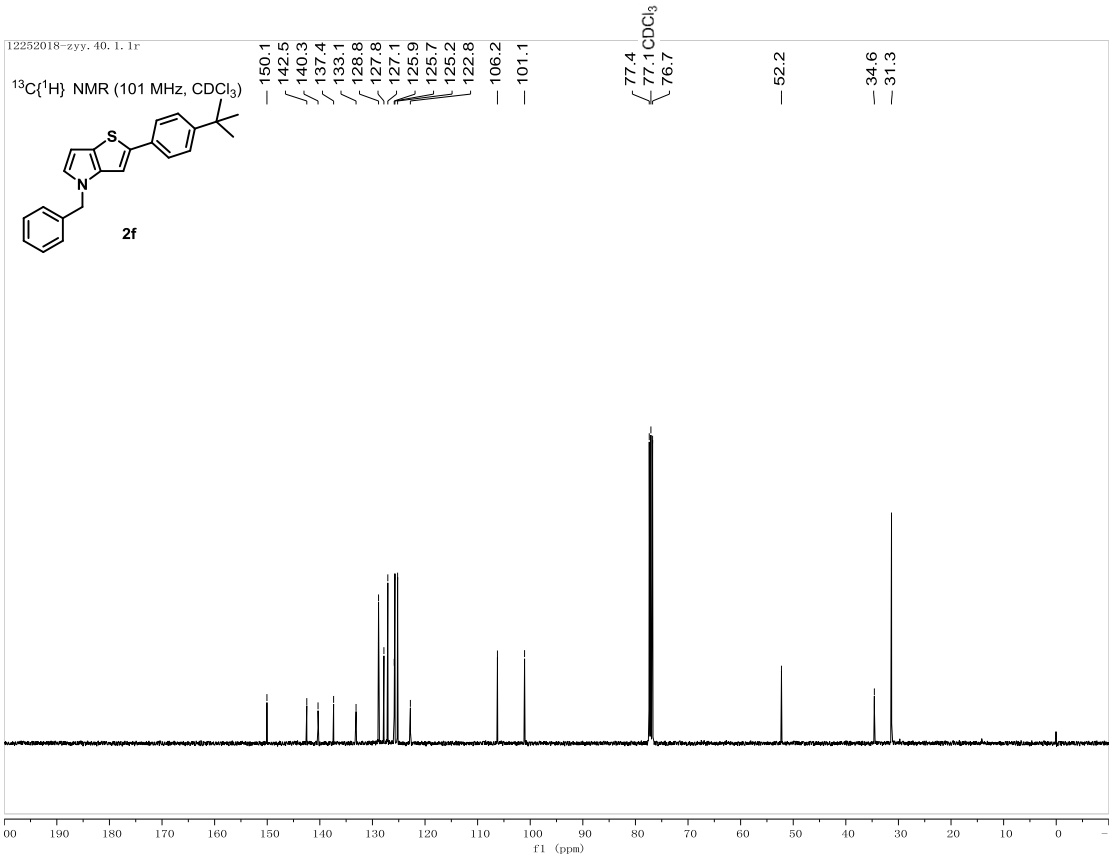

^{1}H NMR (400 MHz, $CDCl_3$)
2d

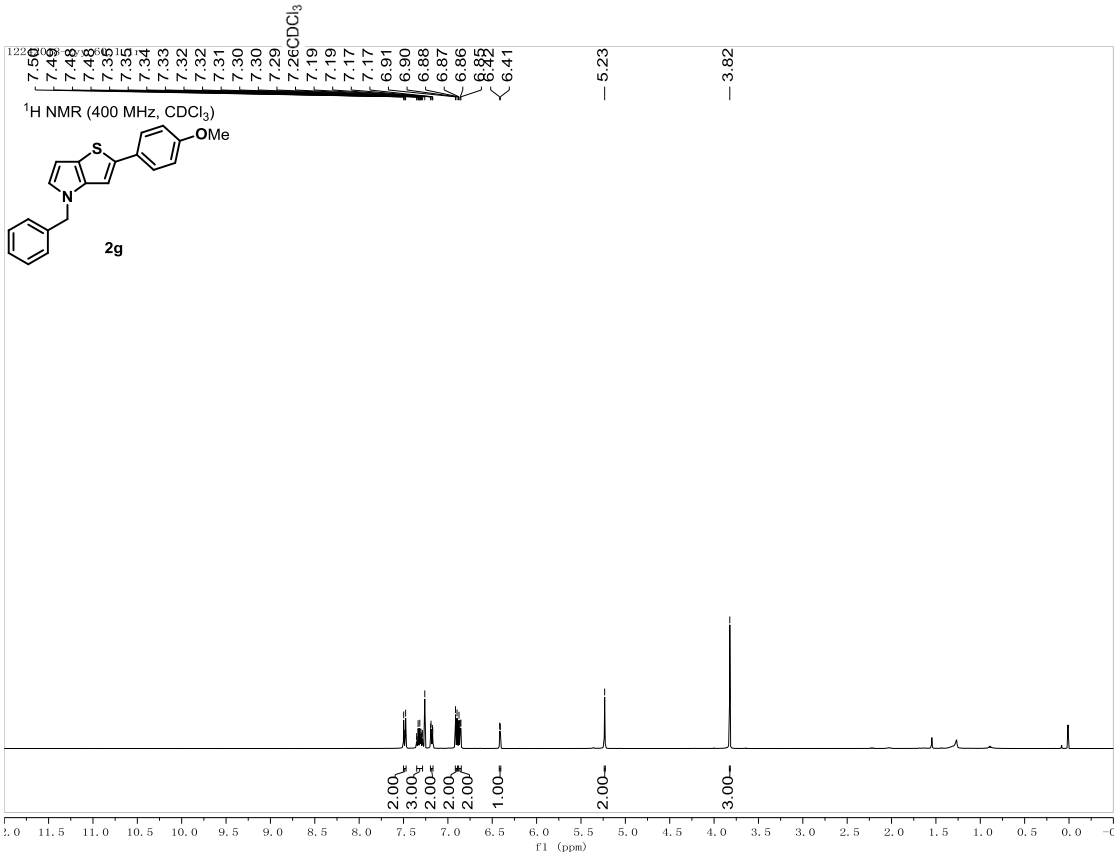

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)
2d

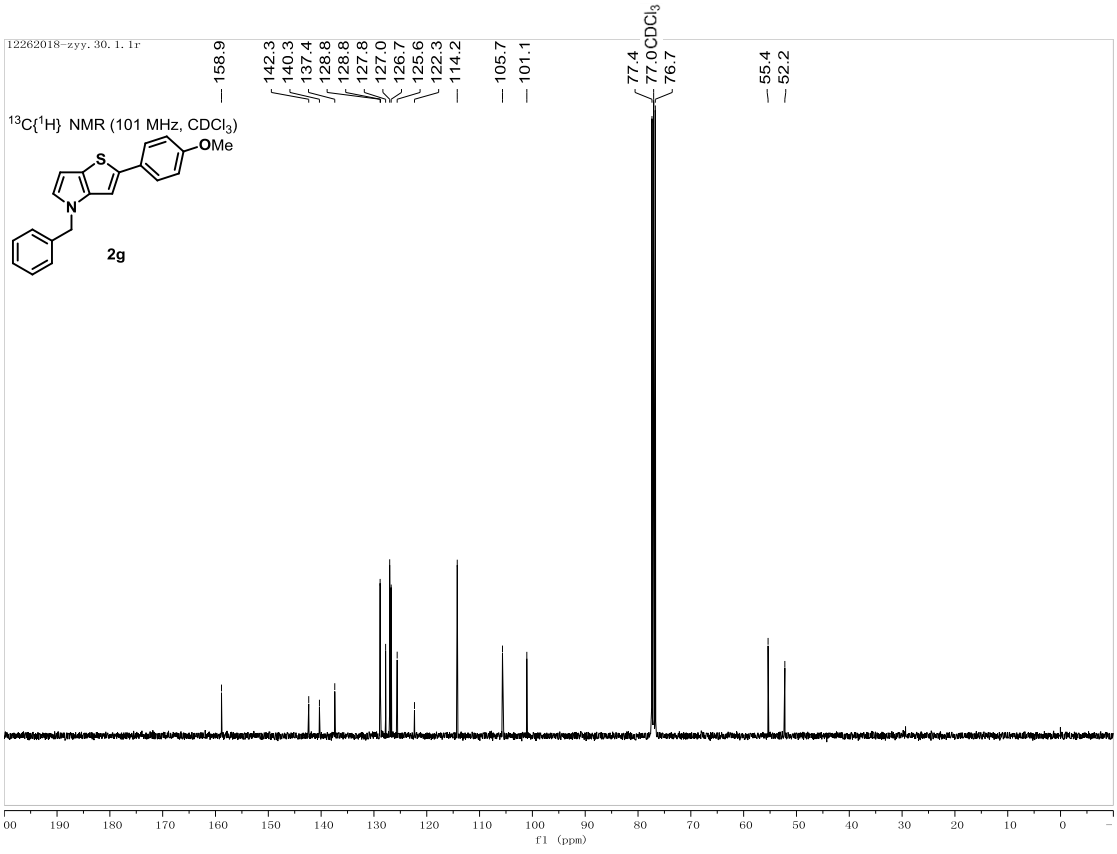

^{1}H NMR (400 MHz, $CDCl_3$)
2e
f1 (ppm)

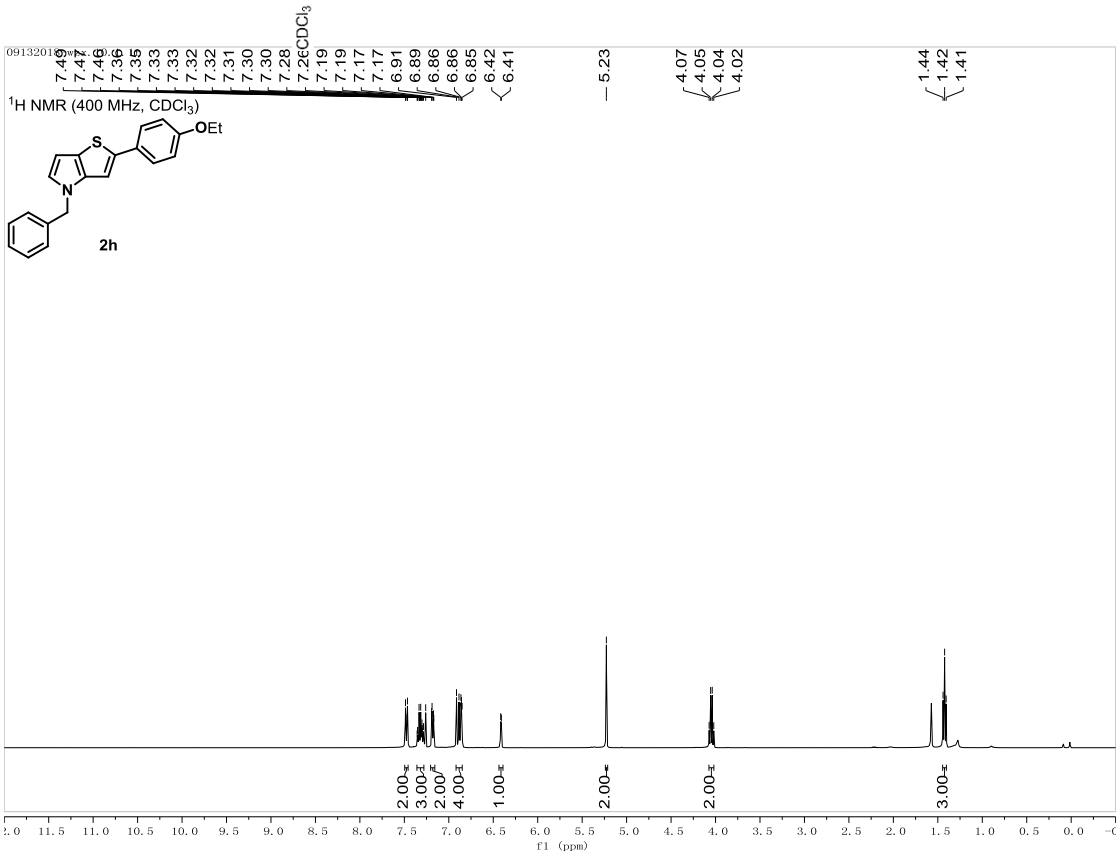

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
2e
f1 (ppm)

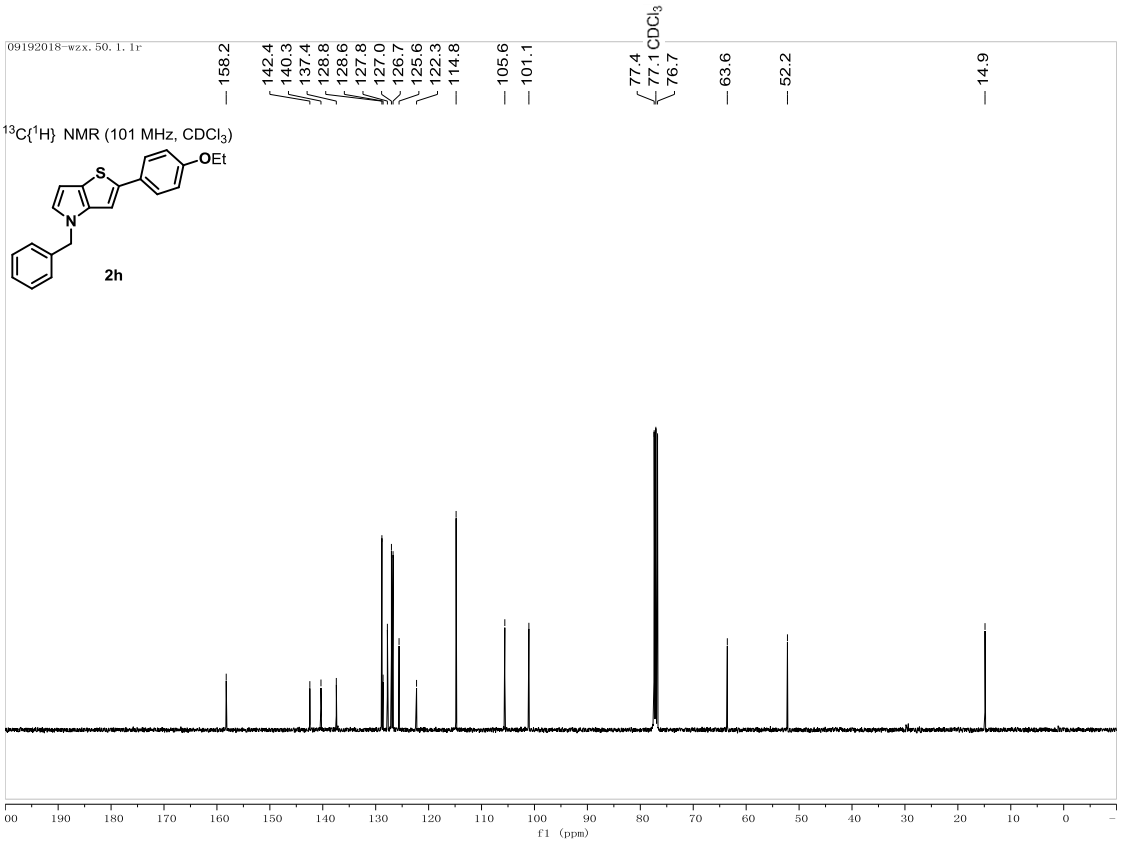

1H NMR (400 MHz, CDCl3)
2f
7.26CDCl3
5.24
1.34
f1 (ppm)

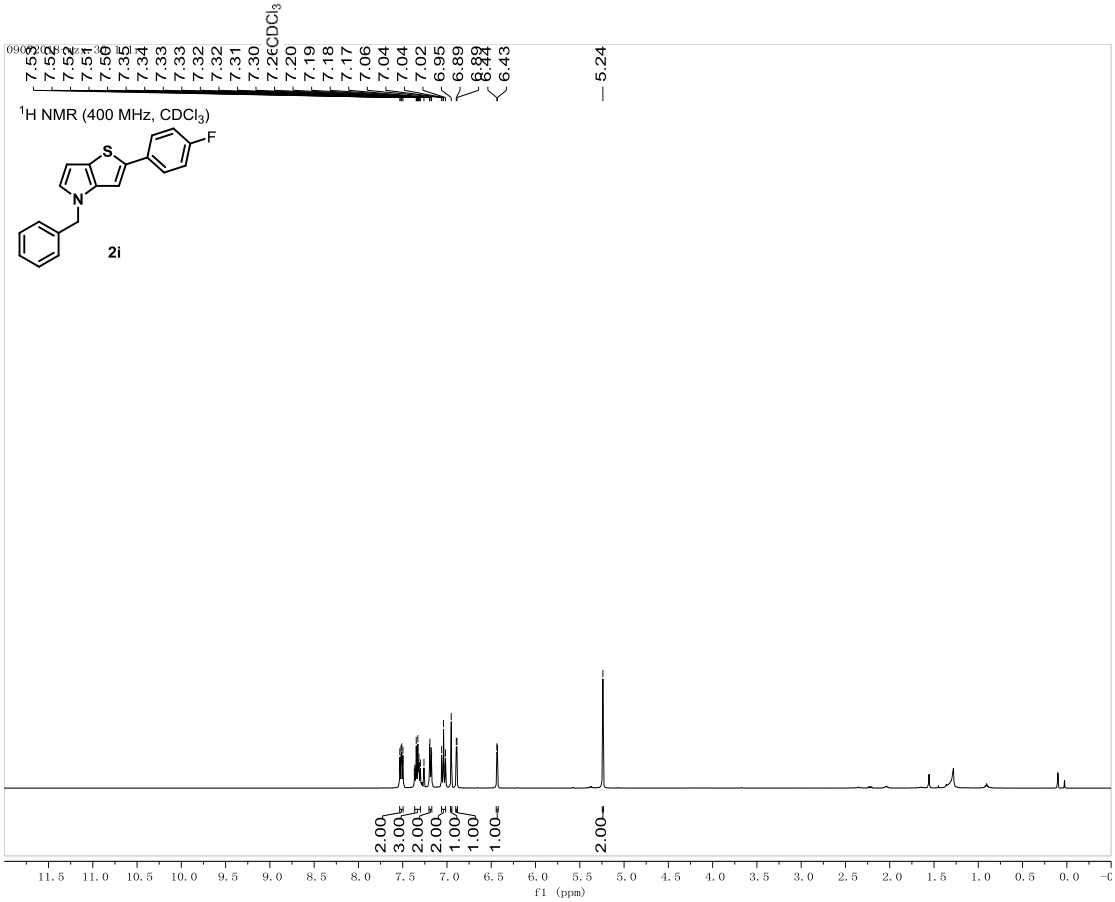

13C{1H} NMR (101 MHz, CDCl3)
2f
150.1
142.5
140.3
137.4
133.1
128.8
127.8
127.1
125.9
125.7
125.2
122.8
106.2
101.1
77.4
77.1CDCl3
76.7
52.2
34.6
31.3
f1 (ppm)

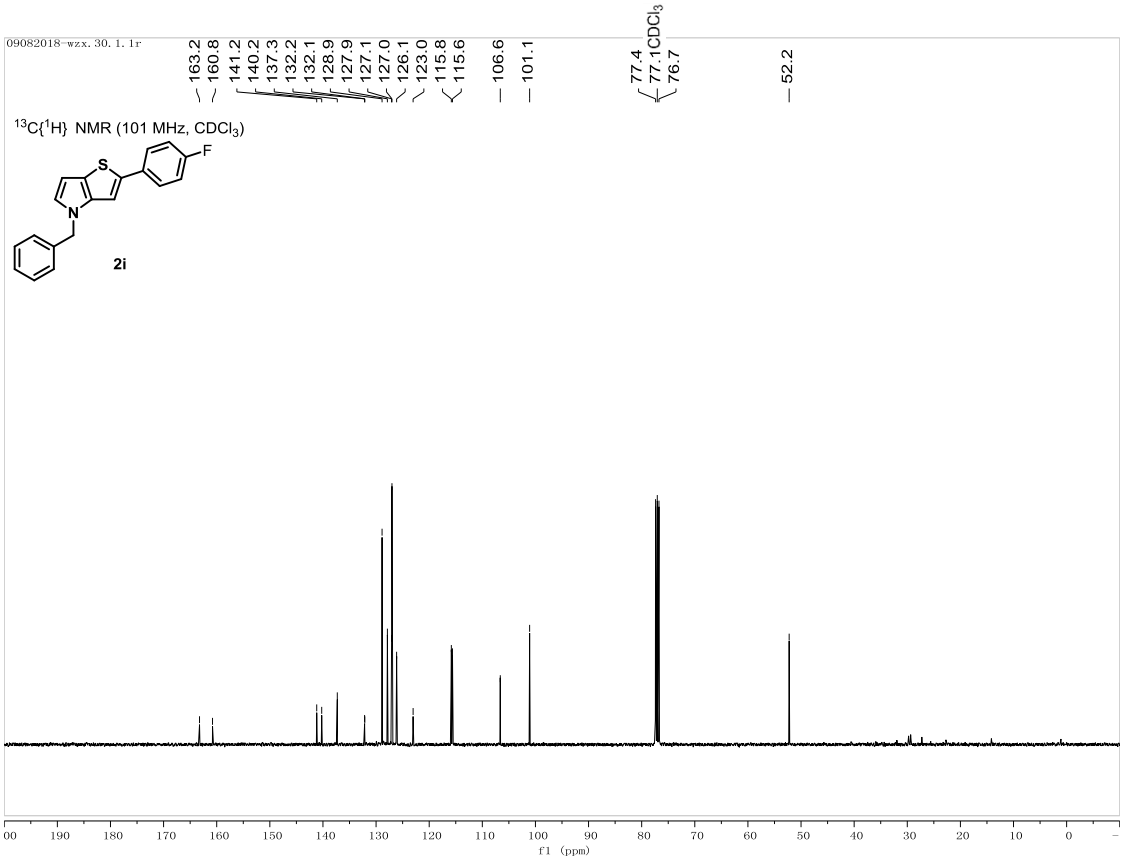

^{1}H NMR (400 MHz, $CDCl_3$)
OMe
S
N
2g
7.50
7.49
7.48
7.46
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.26$CDCl_3$
7.19
7.19
7.17
7.17
6.91
6.90
6.88
6.87
6.86
6.85
6.42
6.41
5.23
3.82
2.00
3.00
2.00
2.00
2.00
1.00
2.00
3.00
f1 (ppm)

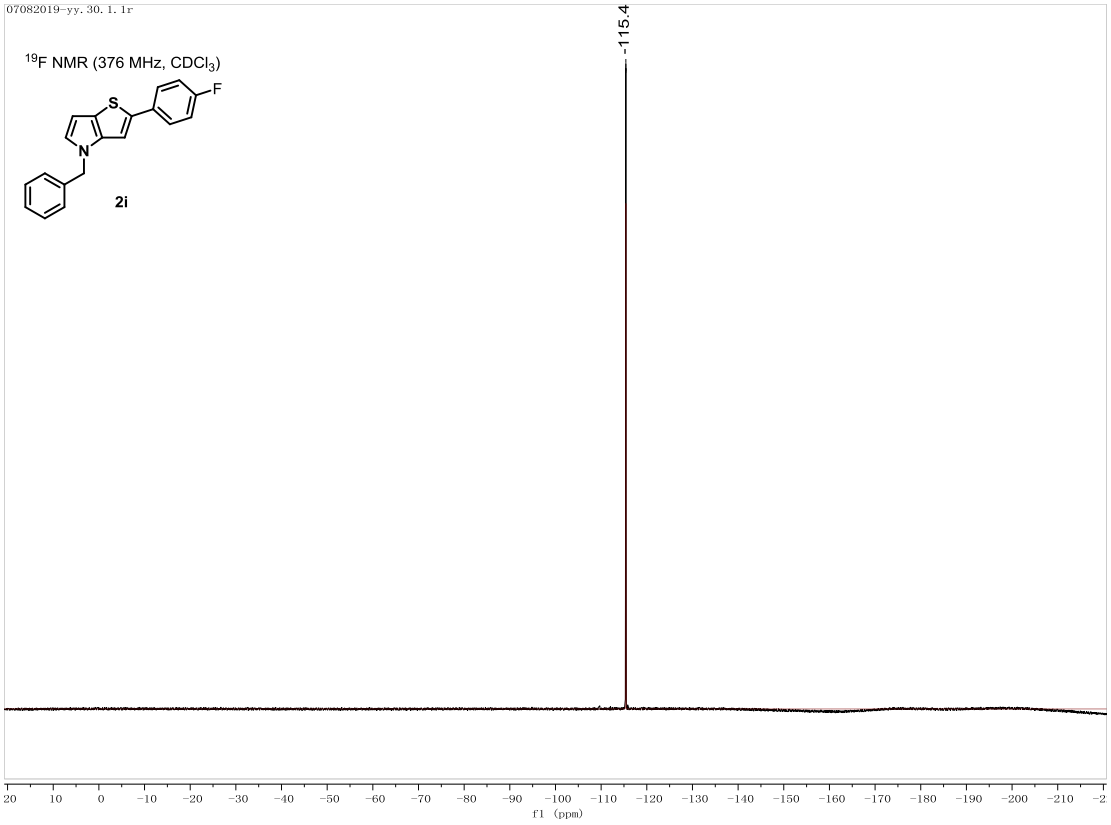

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
OMe
S
N
2g
158.9
142.3
140.3
137.4
128.8
128.8
127.8
127.0
126.7
125.6
122.3
114.2
105.7
101.1
77.4
77.0$CDCl_3$
76.7
55.4
52.2
f1 (ppm)

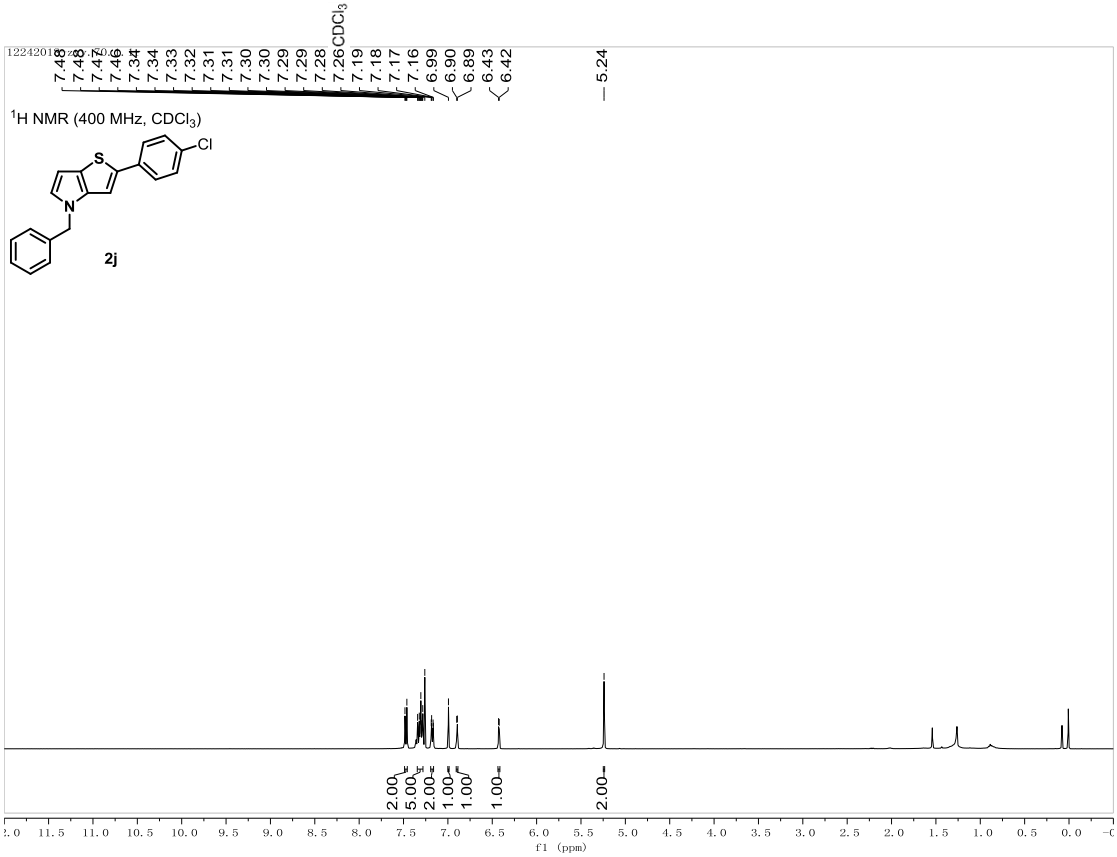

^{1}H NMR (400 MHz, $CDCl_3$)
OEt
S
N
2h
7.49
7.47
7.46
7.36
7.35
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.28
7.26 $CDCl_3$
7.19
7.19
7.17
7.17
6.91
6.89
6.86
6.86
6.85
6.42
6.41
5.23
4.07
4.05
4.04
4.02
1.44
1.42
1.41
2.00
3.00
2.00
4.00
1.00
2.00
2.00
3.00
f1 (ppm)

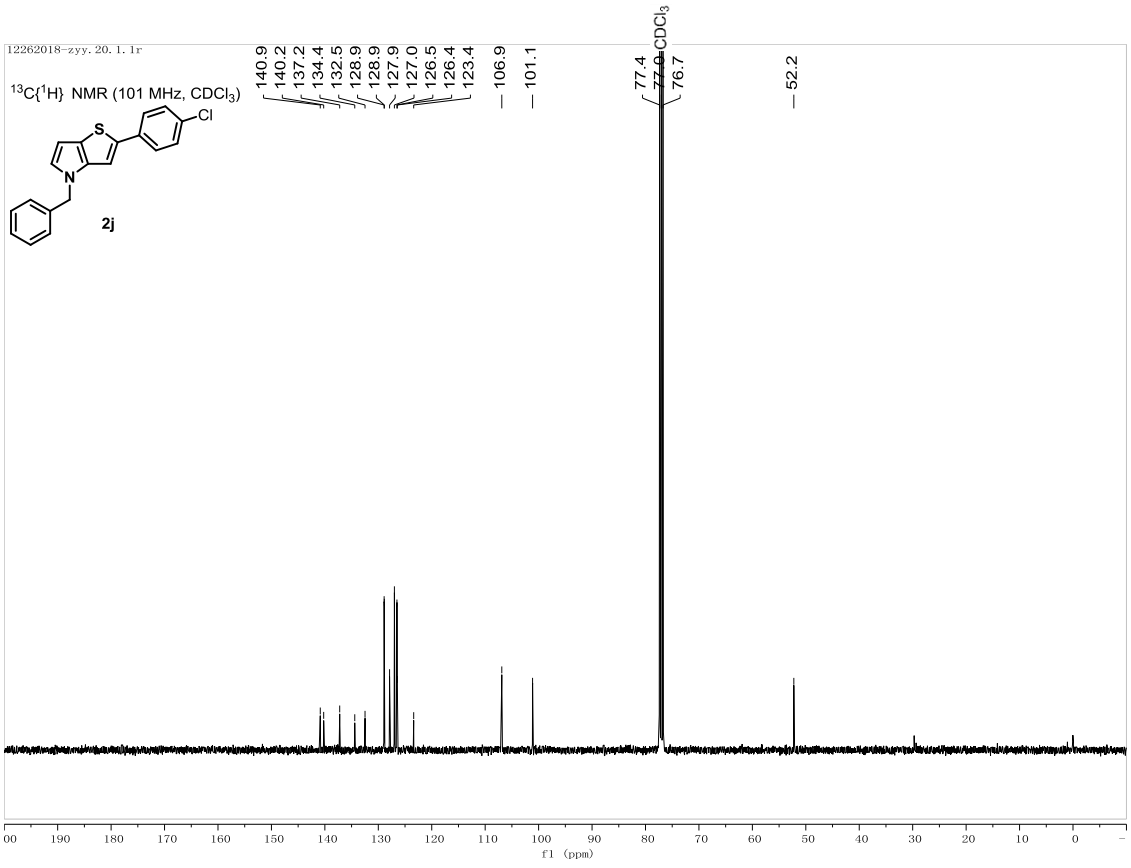

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)
OEt
S
N
2h
158.2
142.4
140.3
137.4
128.8
128.6
127.8
127.0
126.7
125.6
122.3
114.8
105.6
101.1
77.4
77.1 $CDCl_3$
76.7
63.6
52.2
14.9
f1 (ppm)

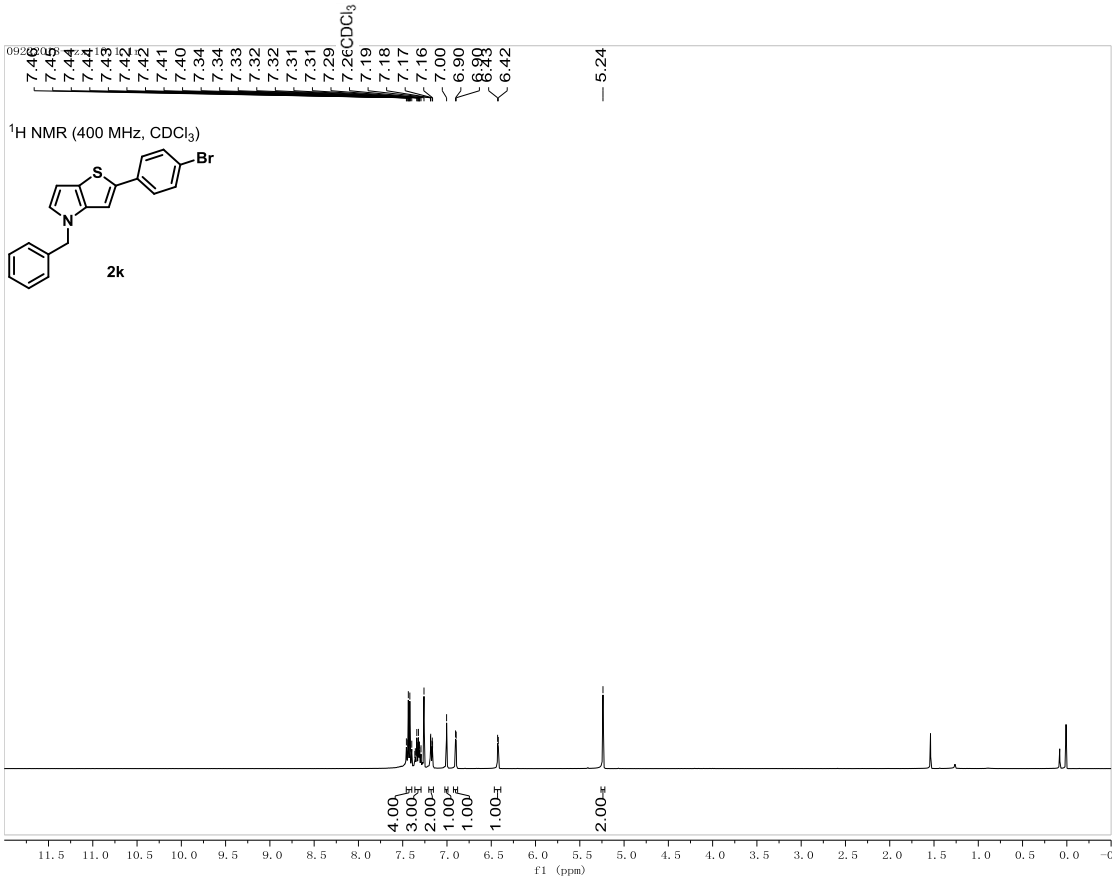

7.55
7.52
7.52
7.51
7.56
7.35
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.26CDCl3
7.20
7.19
7.18
7.17
7.06
7.04
7.04
7.02
6.95
6.89
6.89
6.44
6.43
5.24
1H NMR (400 MHz, CDCl3)
S
F
N
2i
2.00
3.00
2.00
2.00
1.00
1.00
1.00
2.00
f1 (ppm)

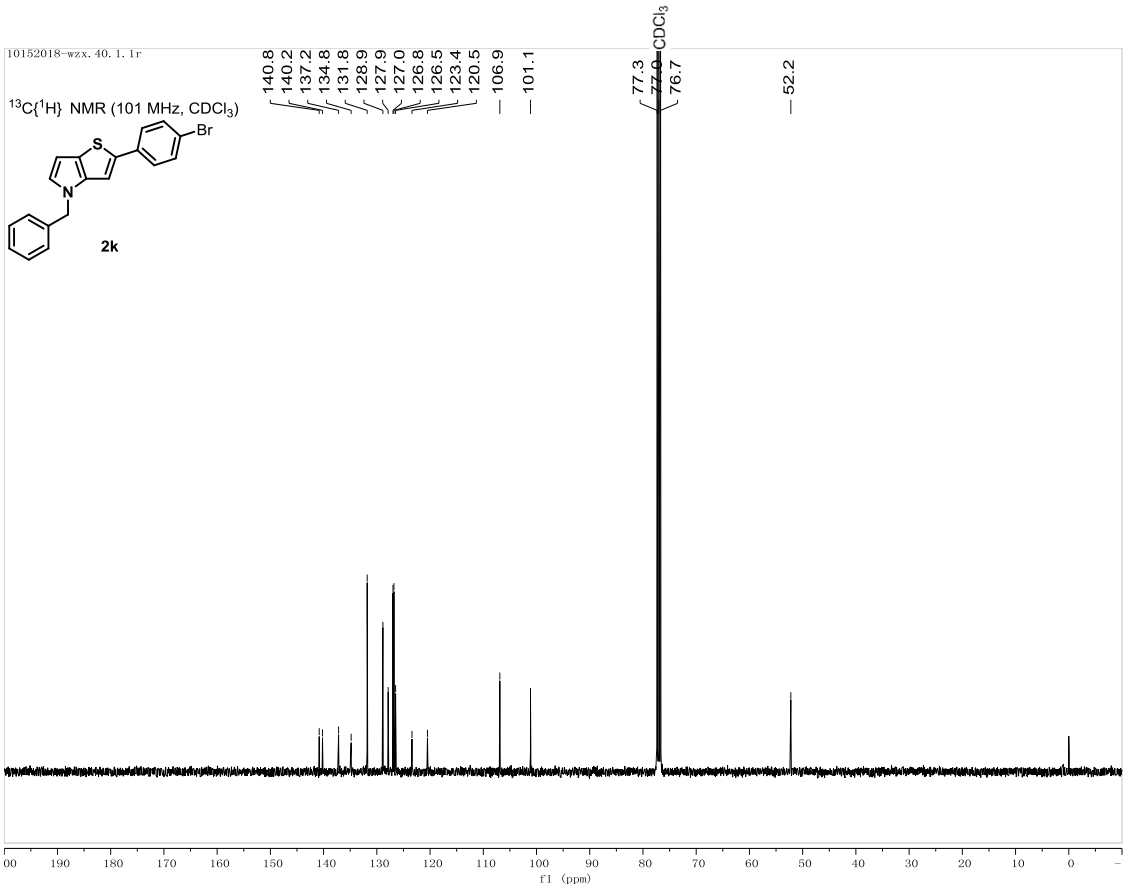

09082018-wzx. 30. 1. 1r
163.2
160.8
141.2
140.2
137.3
132.2
132.1
128.9
127.9
127.1
127.0
126.1
123.0
115.8
115.6
106.6
101.1
77.4
77.1CDCl3
76.7
52.2
13C{1H} NMR (101 MHz, CDCl3)
S
F
N
2i
f1 (ppm)

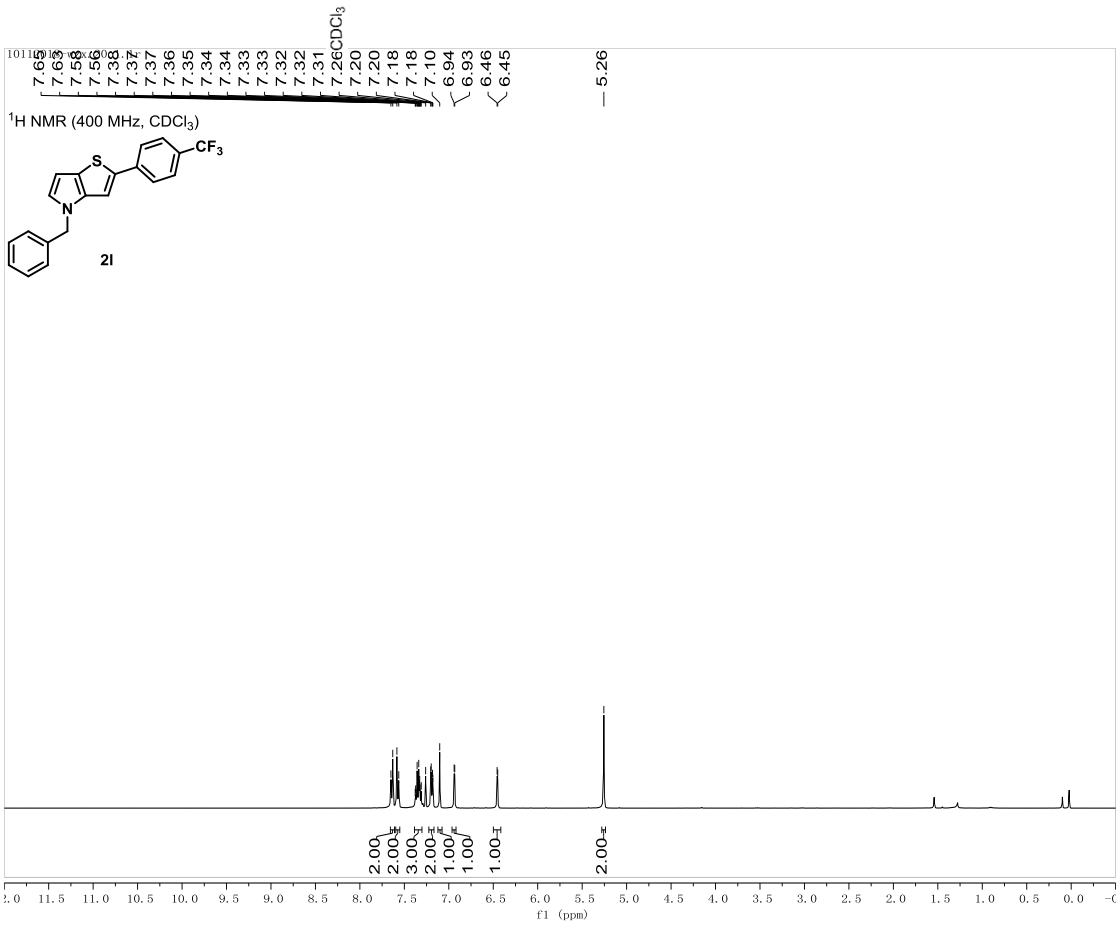

07082019-yy. 30. 1. 1r
^{19}F NMR (376 MHz, $CDCl_3$)
S
F
N
2i
-115.4
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 −2
f1 (ppm)


^{1}H NMR (400 MHz, $CDCl_3$)
2j
7.48
7.47
7.46
7.34
7.33
7.32
7.31
7.30
7.29
7.28
7.26 $CDCl_3$
7.19
7.18
7.17
7.16
6.99
6.90
6.89
6.43
6.42
5.24
2.00
5.00
2.00
1.00
1.00
2.00
f1 (ppm)

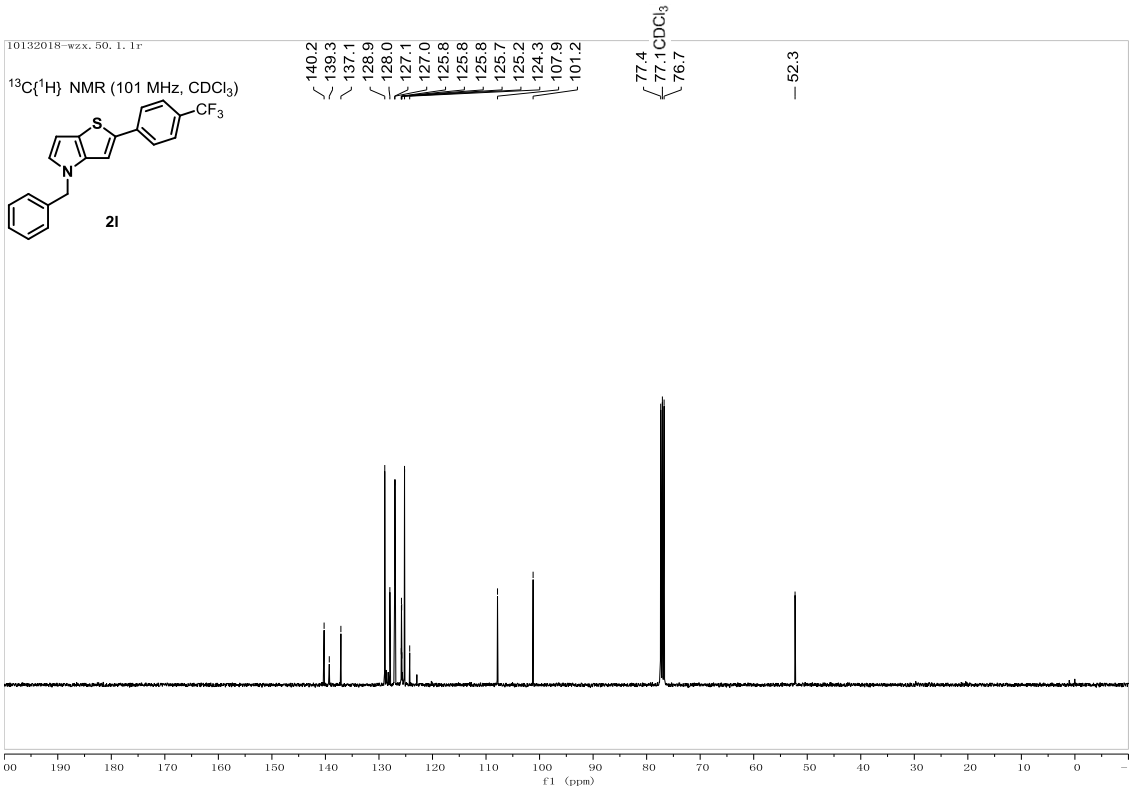

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)
2j
140.9
140.2
137.2
134.4
132.5
128.9
128.9
127.9
127.0
126.5
126.4
123.4
106.9
101.1
77.4
77.0 $CDCl_3$
76.7
52.2
f1 (ppm)


^{1}H NMR (400 MHz, CDCl$_3$)
Br
S
N
2k
CDCl$_3$
7.45
7.44
7.44
7.43
7.42
7.42
7.41
7.40
7.34
7.34
7.33
7.32
7.32
7.31
7.31
7.29
7.26
7.19
7.18
7.17
7.16
7.00
6.90
6.90
6.43
6.42
5.24
4.00
3.00
2.00
1.00
1.00
1.00
2.00
f1 (ppm)

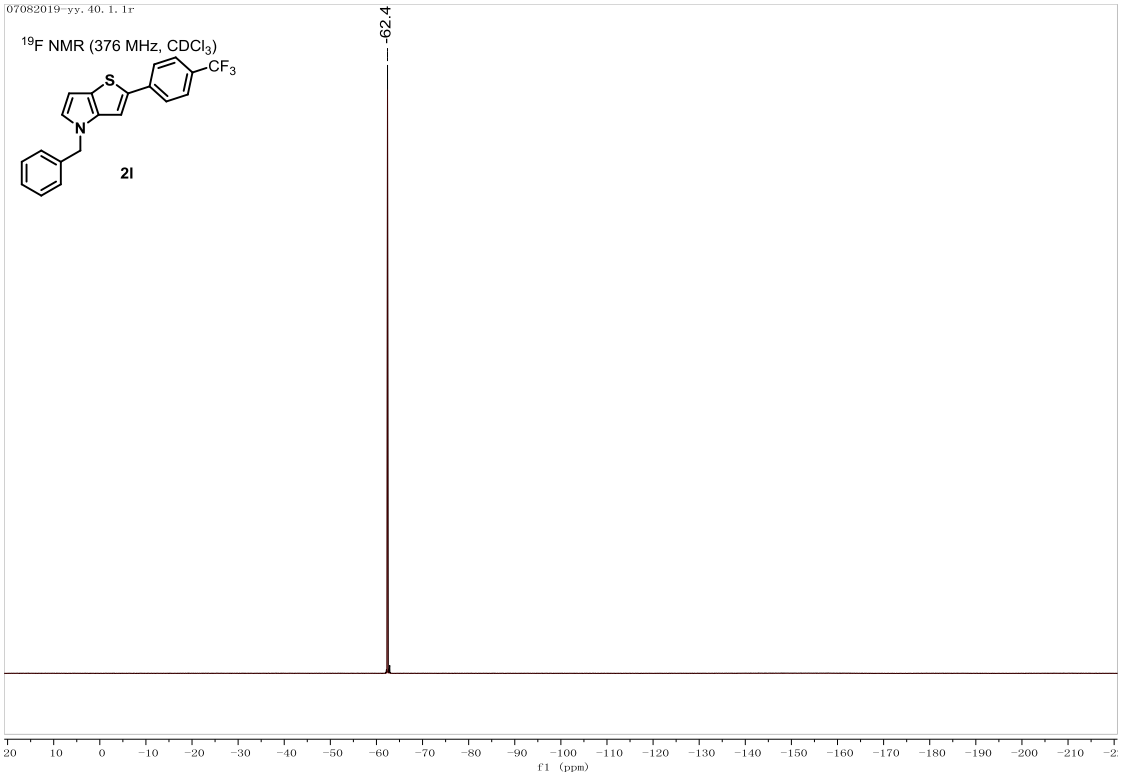

10152018-wzx.40.1.1r
^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)
Br
S
N
2k
CDCl$_3$
140.8
140.2
137.2
134.8
131.8
128.9
127.9
127.0
126.8
126.5
123.4
120.5
106.9
101.1
77.3
77.0
76.7
52.2
f1 (ppm)

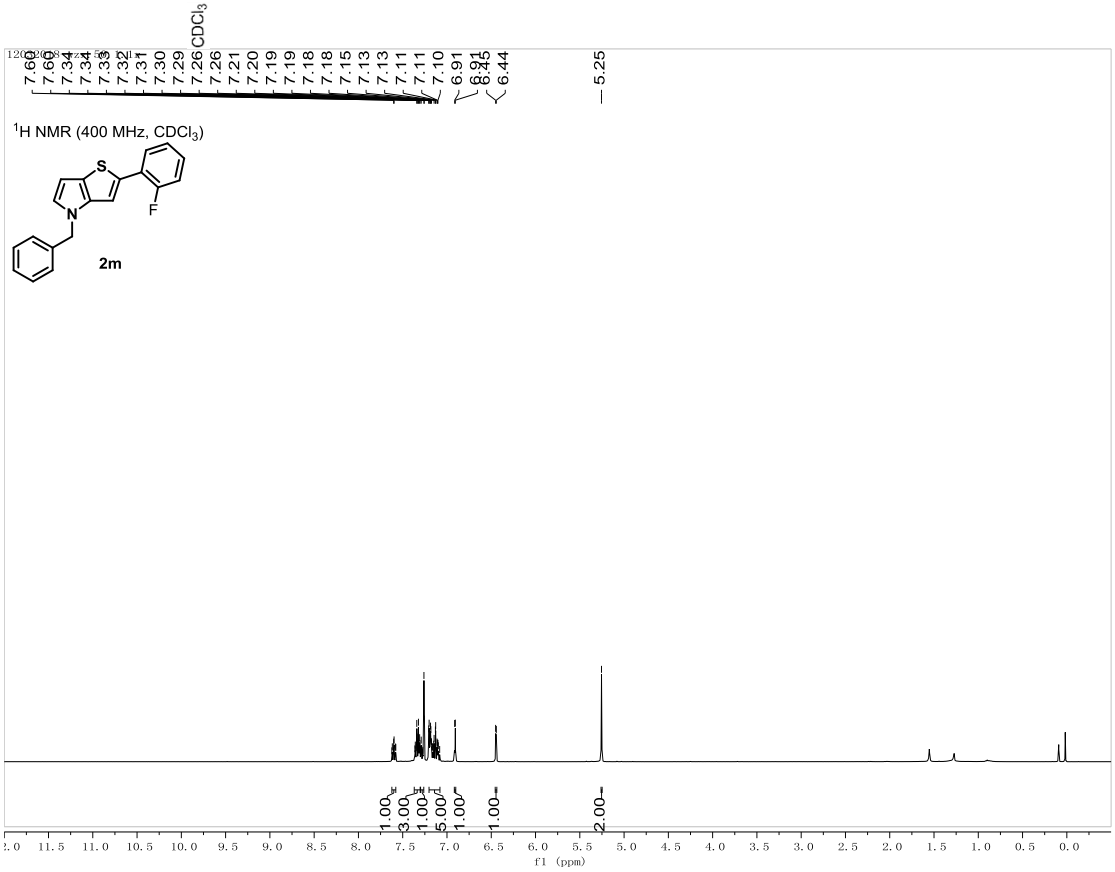


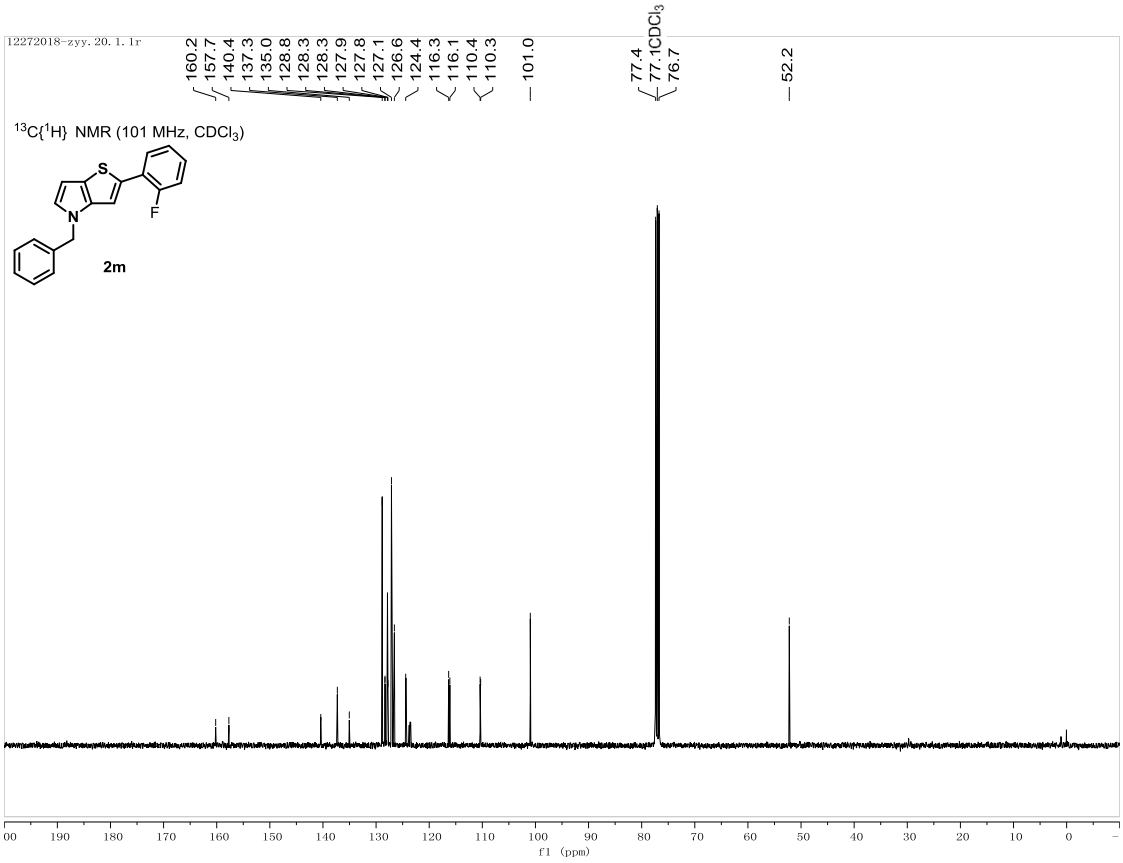
7.66
7.63
7.58
7.56
7.38
7.37
7.37
7.36
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.26CDCl3
7.20
7.20
7.18
7.18
7.10
6.94
6.93
6.46
6.45
5.26
1H NMR (400 MHz, CDCl3)
CF3
S
N
2l
2.00
2.00
3.00
2.00
1.00
1.00
1.00
2.00
f1 (ppm)

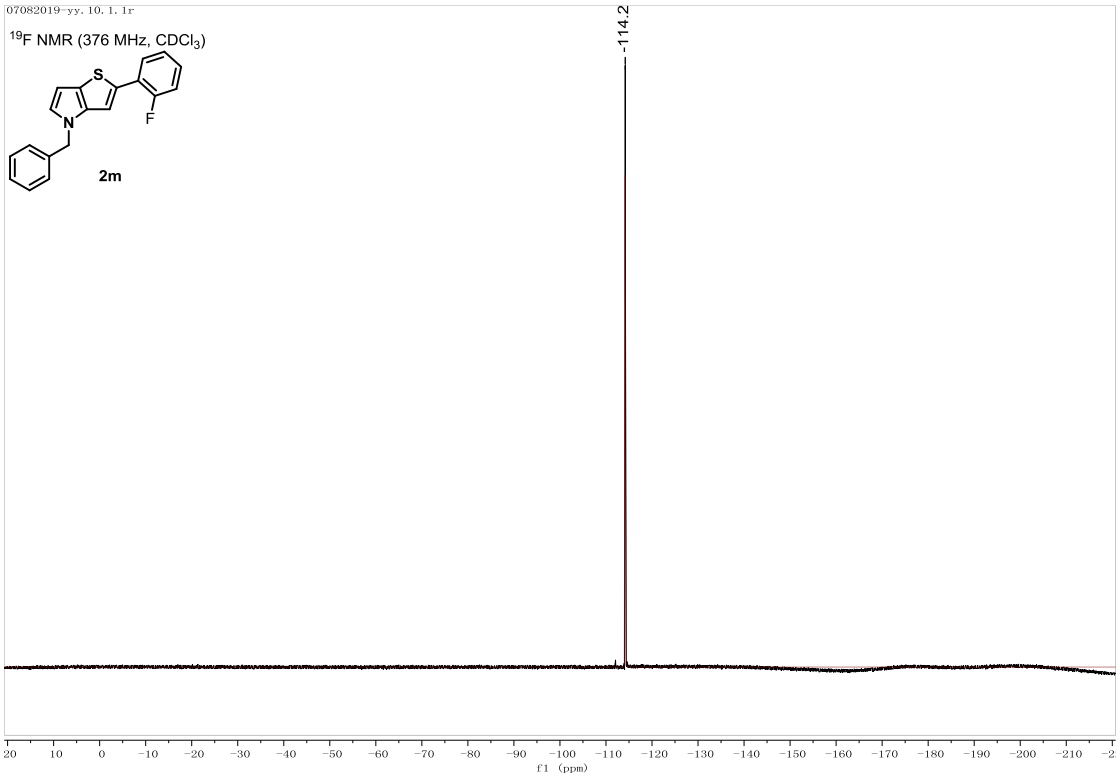


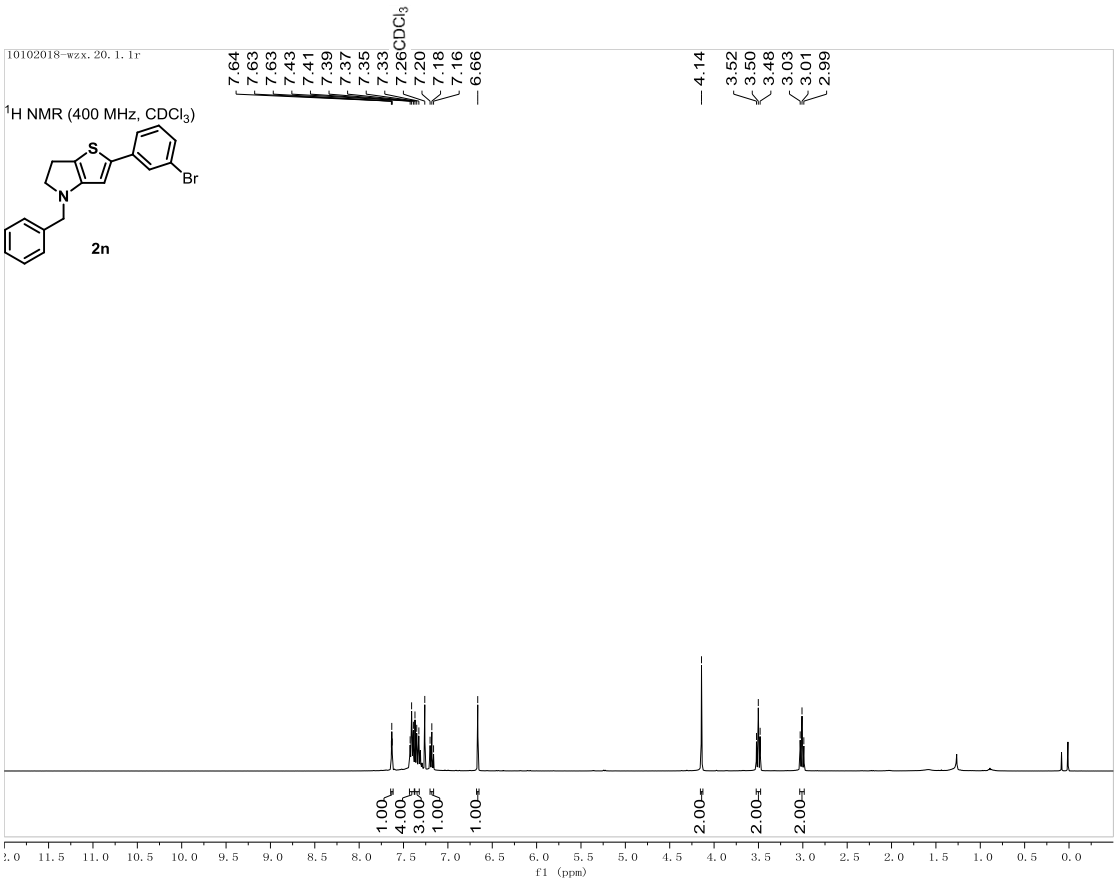
10132018-wzx.50.1.1r
13C{1H} NMR (101 MHz, CDCl3)
CF3
S
N
2l
140.2
139.3
137.1
128.9
128.0
127.1
127.0
125.8
125.8
125.7
125.2
124.3
107.9
101.2
77.4
77.1CDCl3
76.7
52.3
f1 (ppm)

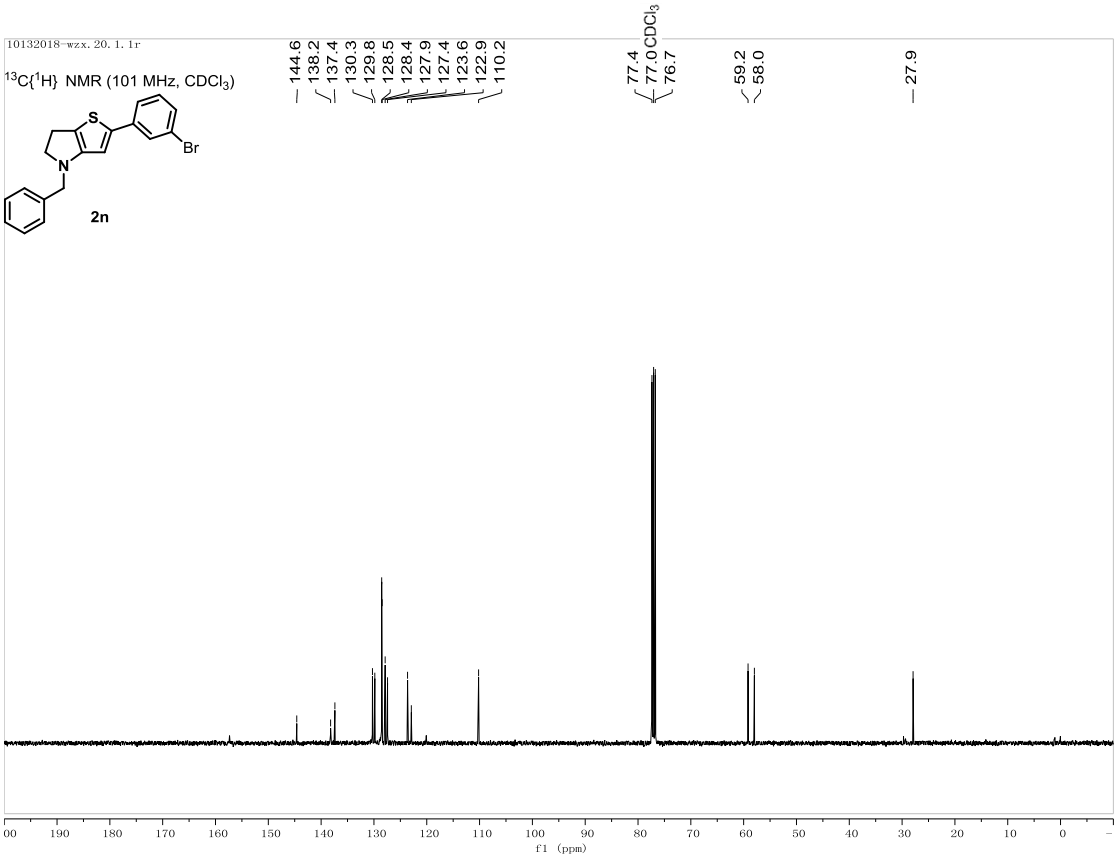

07082019-yy. 40. 1. 1r
^{19}F NMR (376 MHz, CDCl$_3$)
CF$_3$
S
N
2l
-62.4
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

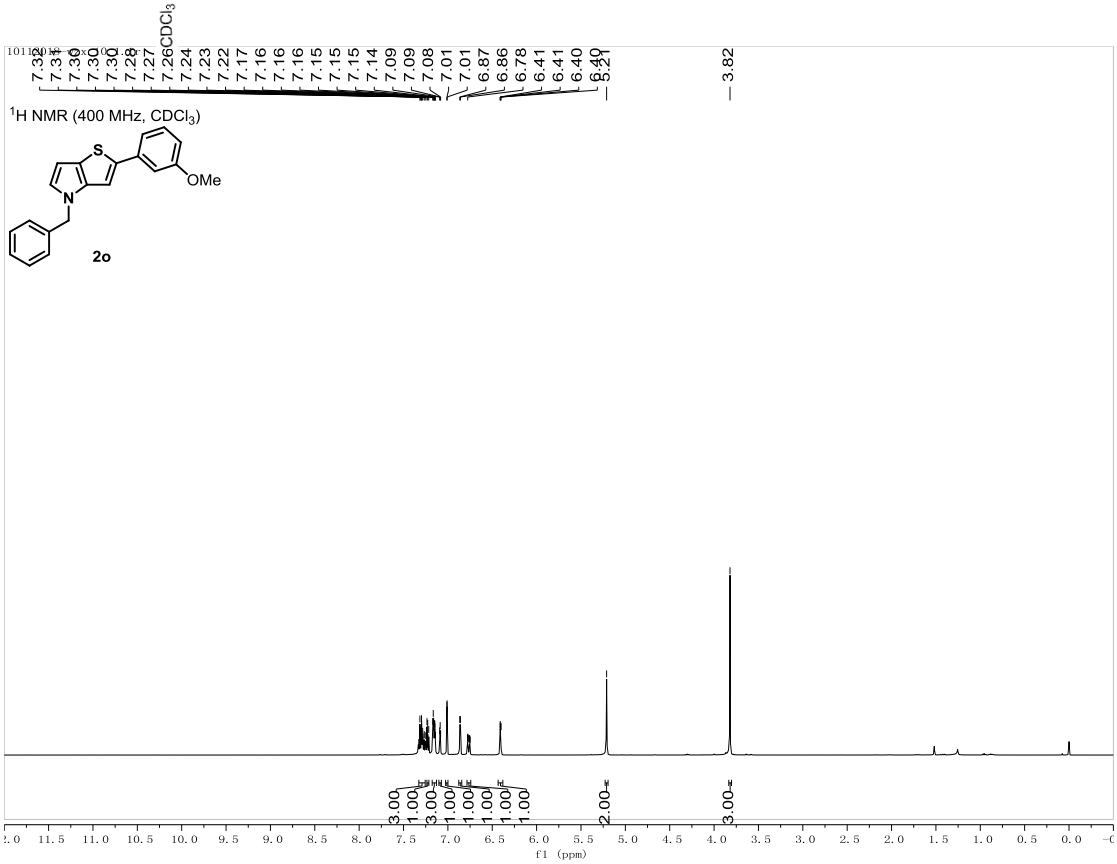

7.60
7.60
7.34
7.34
7.33
7.32
7.31
7.30
7.29
7.26 CDCl3
7.21
7.20
7.19
7.19
7.18
7.15
7.13
7.11
7.11
7.10
6.91
6.91
6.45
6.44
5.25
1H NMR (400 MHz, CDCl3)
S
N
F
2m
1.00
3.00
1.00
5.00
1.00
1.00
2.00
f1 (ppm)

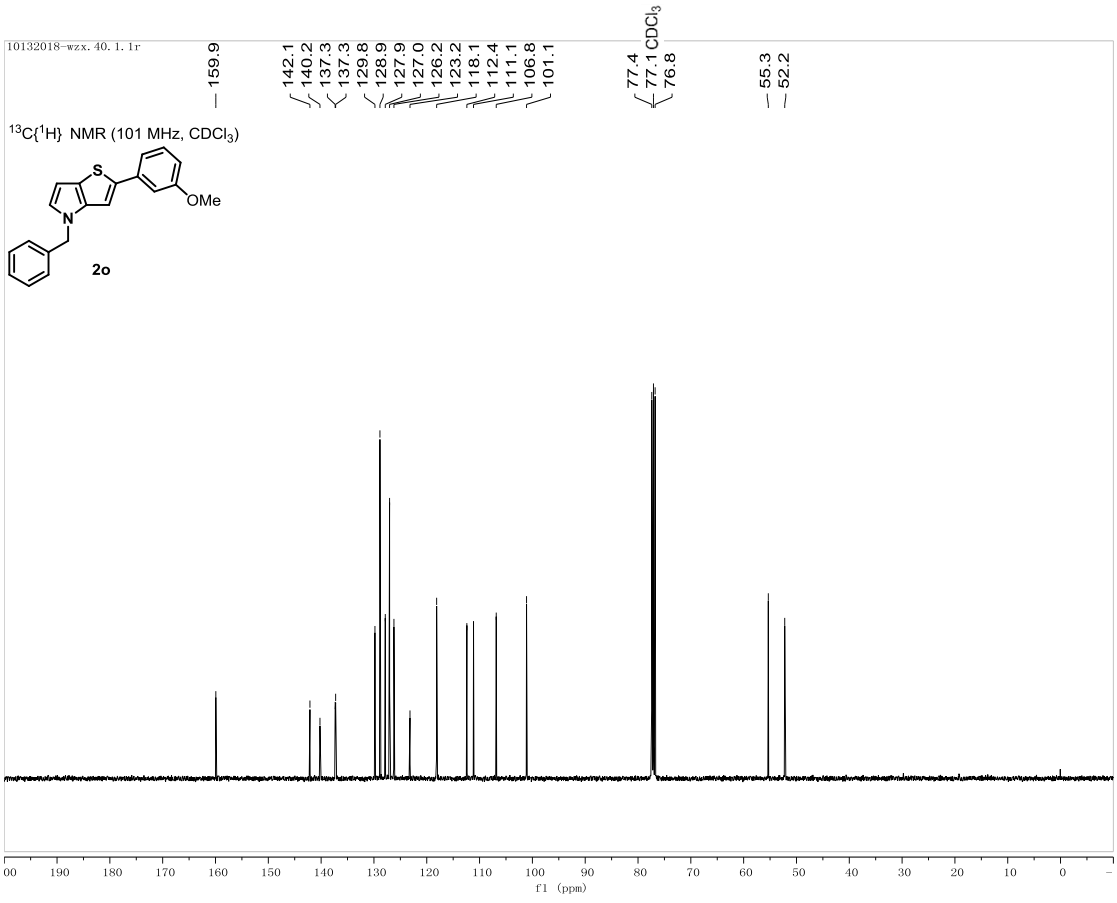

12272018-zyy.20.1.1r
160.2
157.7
140.4
137.3
135.0
128.8
128.3
128.3
127.9
127.8
127.1
126.6
124.4
116.3
116.1
110.4
110.3
101.0
77.4
77.1 CDCl3
76.7
52.2
13C{1H} NMR (101 MHz, CDCl3)
S
N
F
2m
f1 (ppm)

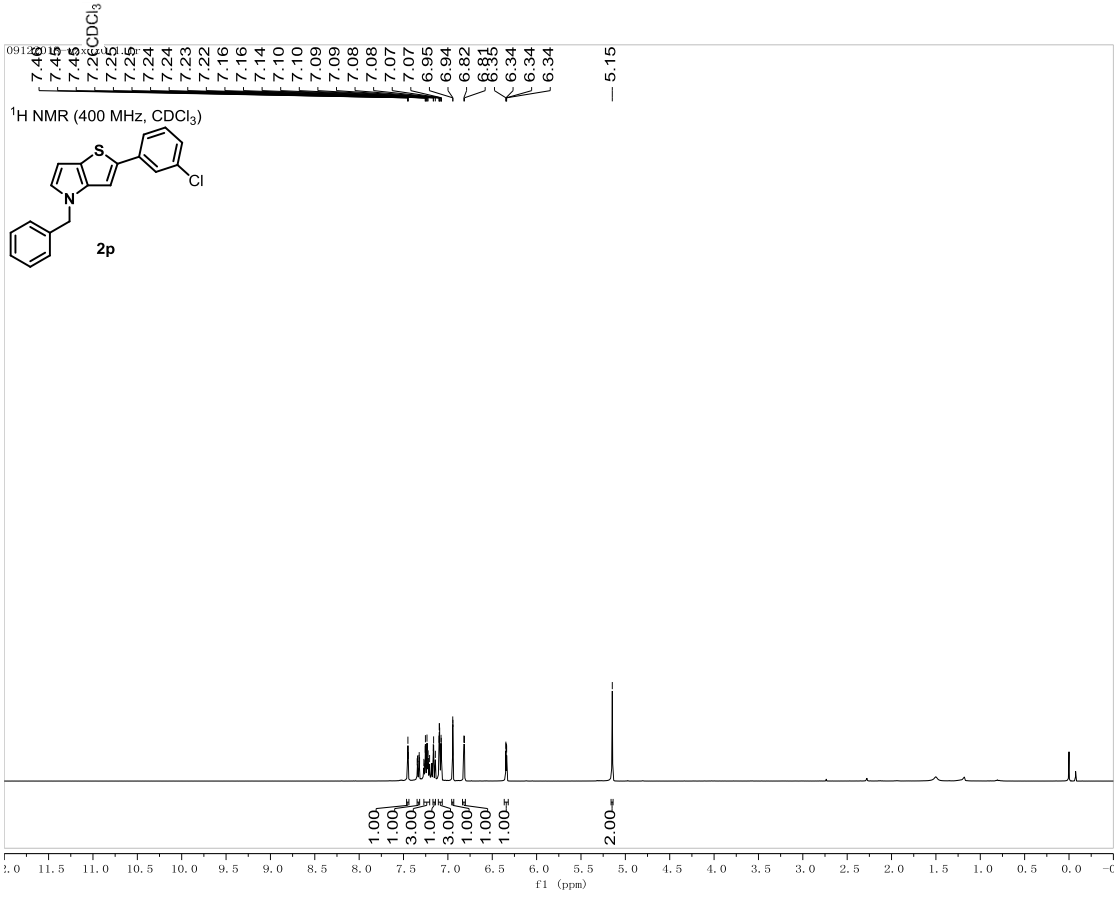

07082019-yy. 10. 1. 1r
^{19}F NMR (376 MHz, CDCl$_3$)
S
N
F
2m
-114.2
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

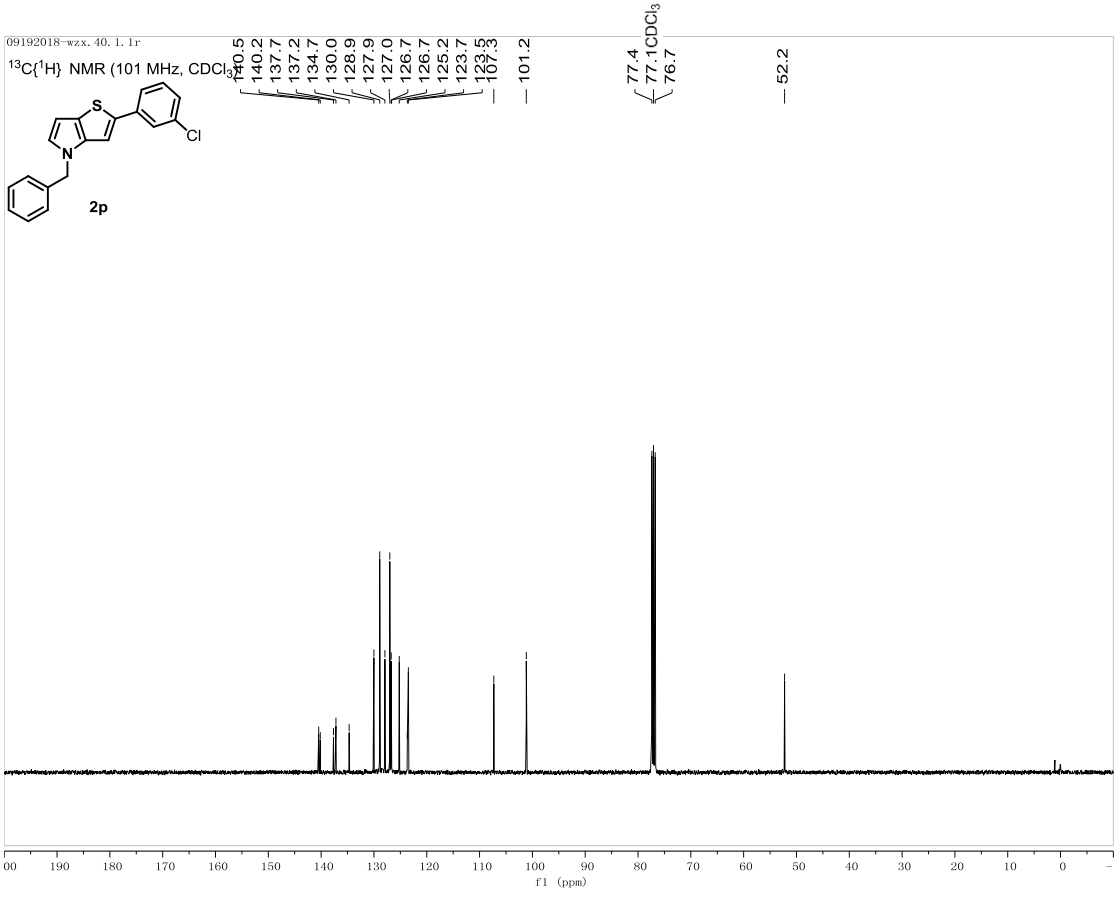

10102018-wzx. 20. 1. 1r
^{1}H NMR (400 MHz, $CDCl_3$)
2n
7.64
7.63
7.63
7.43
7.41
7.39
7.37
7.35
7.33
7.26$CDCl_3$
7.20
7.18
7.16
6.66
4.14
3.52
3.50
3.48
3.03
3.01
2.99
1.00
4.00
3.00
1.00
1.00
2.00
2.00
2.00
f1 (ppm)

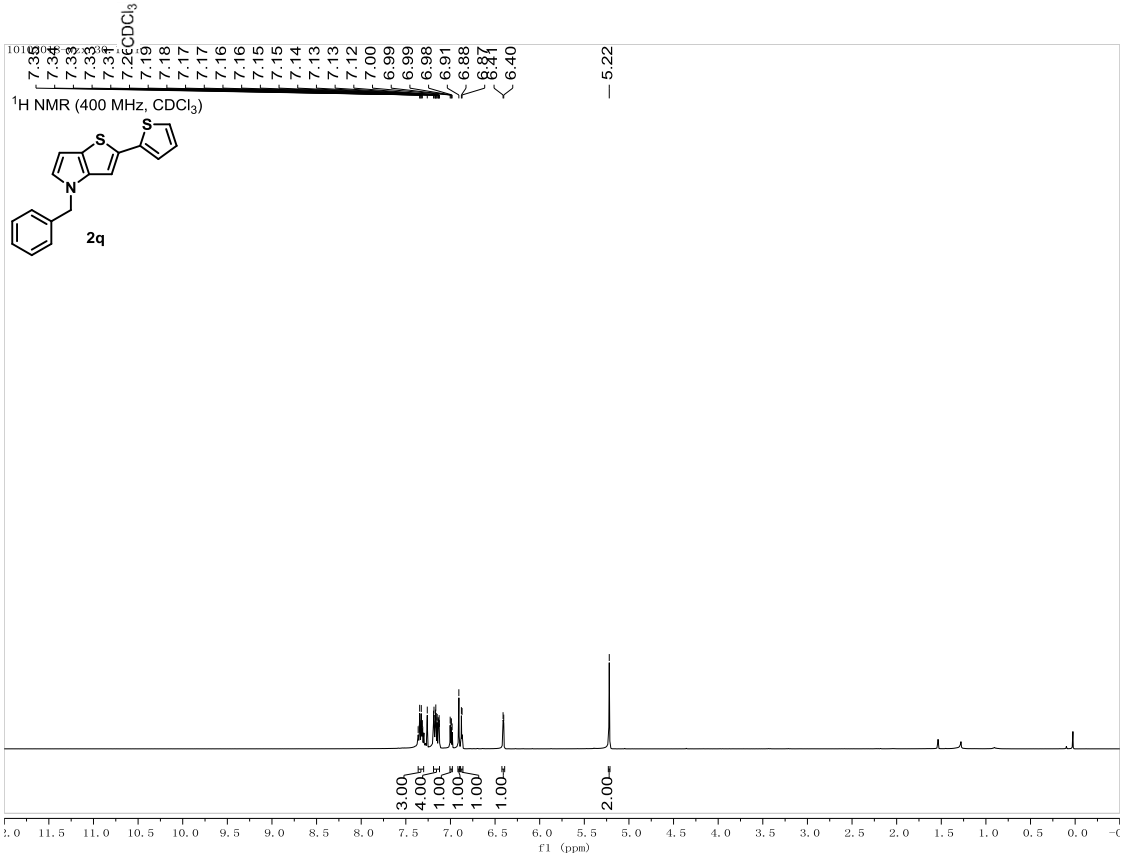

10132018-wzx. 20. 1. 1r
$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
2n
144.6
138.2
137.4
130.3
129.8
128.5
128.4
127.9
127.4
123.6
122.9
110.2
77.4
77.0$CDCl_3$
76.7
59.2
58.0
27.9
f1 (ppm)

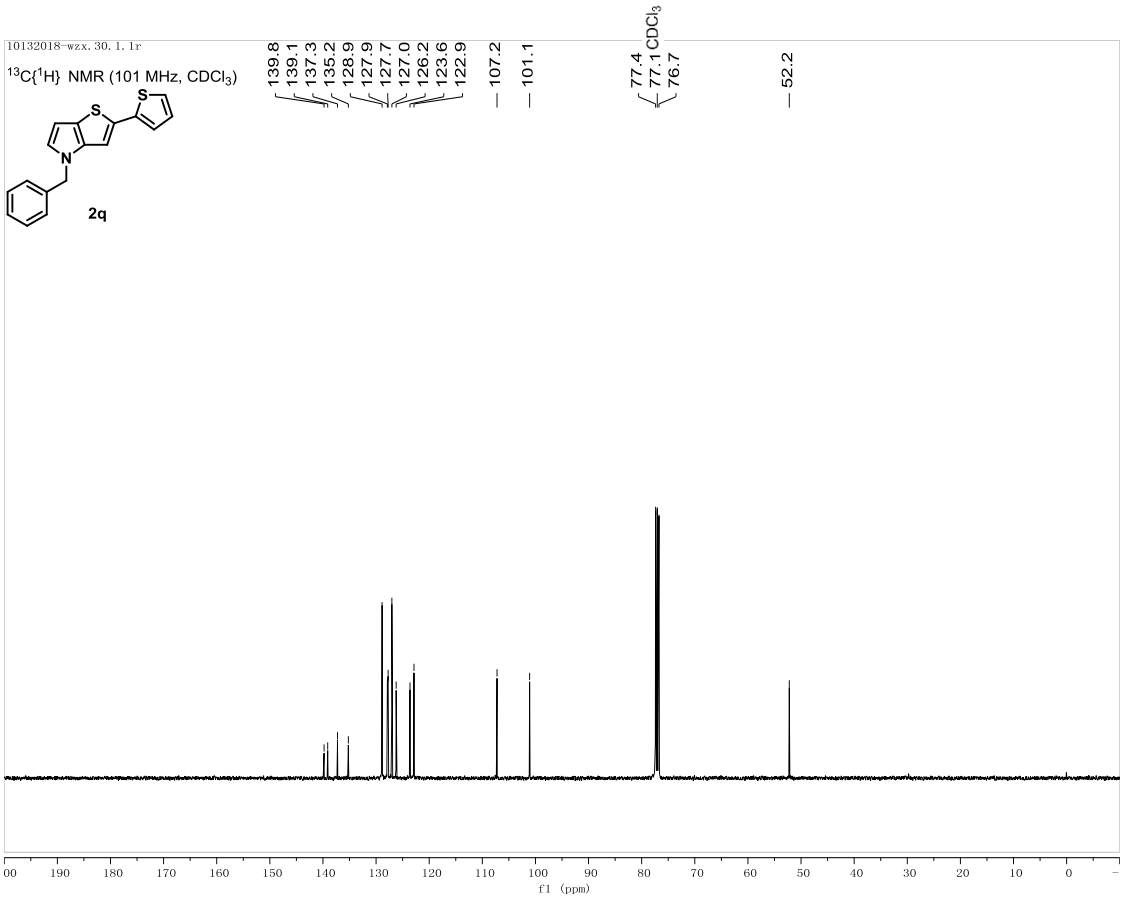

^{1}H NMR (400 MHz, $CDCl_3$)
OMe
2o
f1 (ppm)

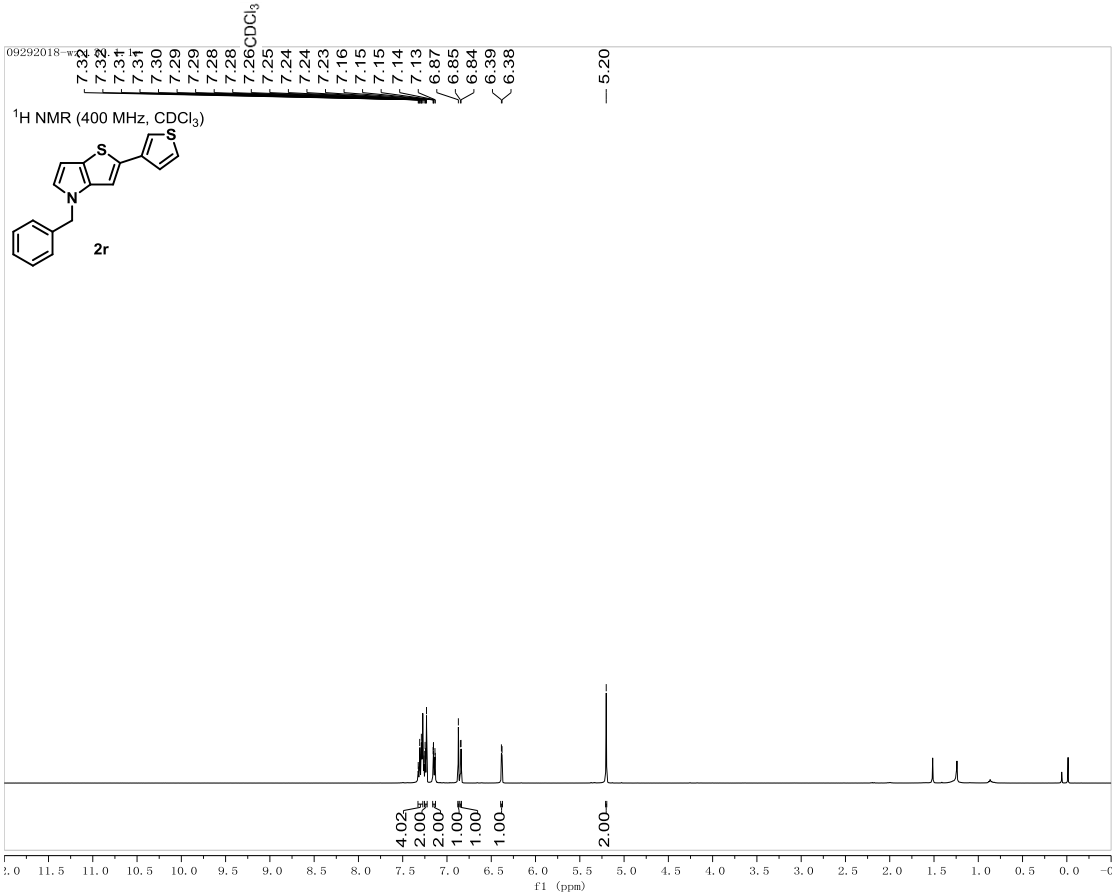

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
OMe
2o
f1 (ppm)


^{1}H NMR (400 MHz, CDCl$_3$)
2p
f1 (ppm)

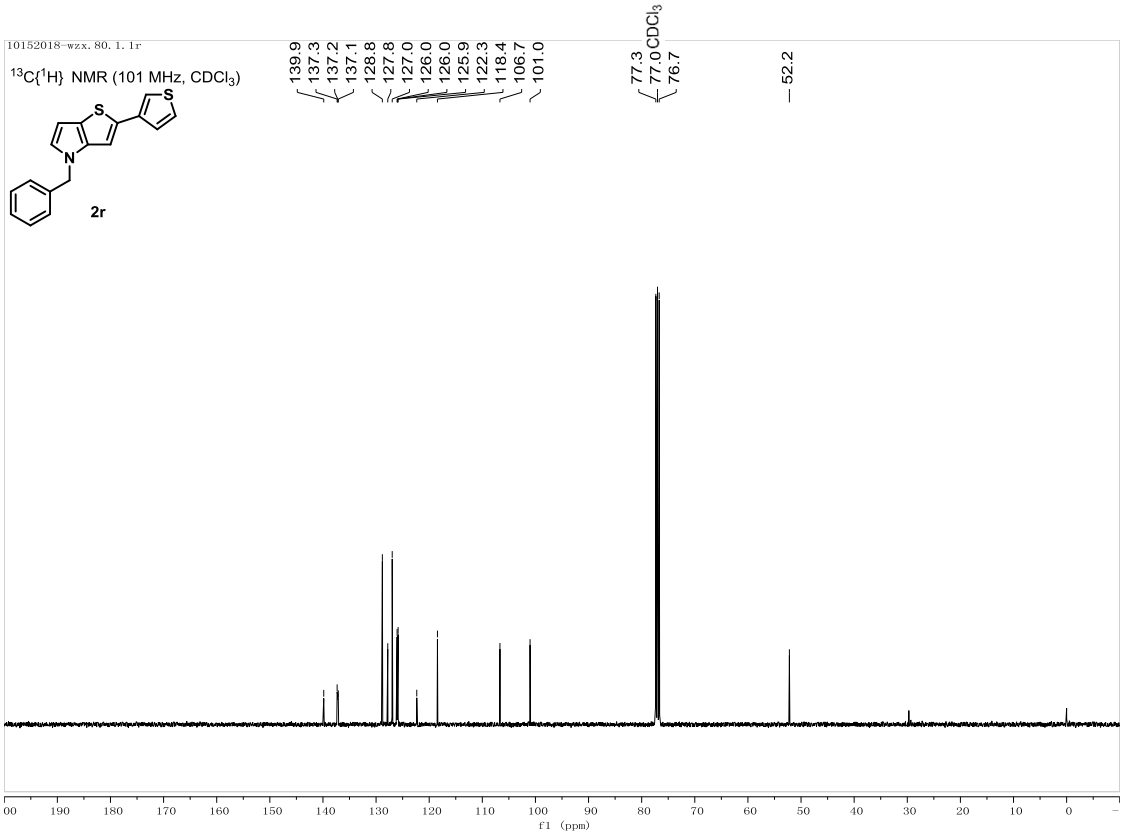

^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)
2p
f1 (ppm)


^{1}H NMR (400 MHz, CDCl$_3$)
2q
7.35
7.34
7.33
7.33
7.31
7.26 CDCl$_3$
7.19
7.18
7.17
7.17
7.16
7.16
7.15
7.15
7.14
7.13
7.13
7.12
7.00
6.99
6.99
6.98
6.91
6.88
6.87
6.41
6.40
5.22
3.00
4.00
1.00
1.00
1.00
1.00
2.00
f1 (ppm)

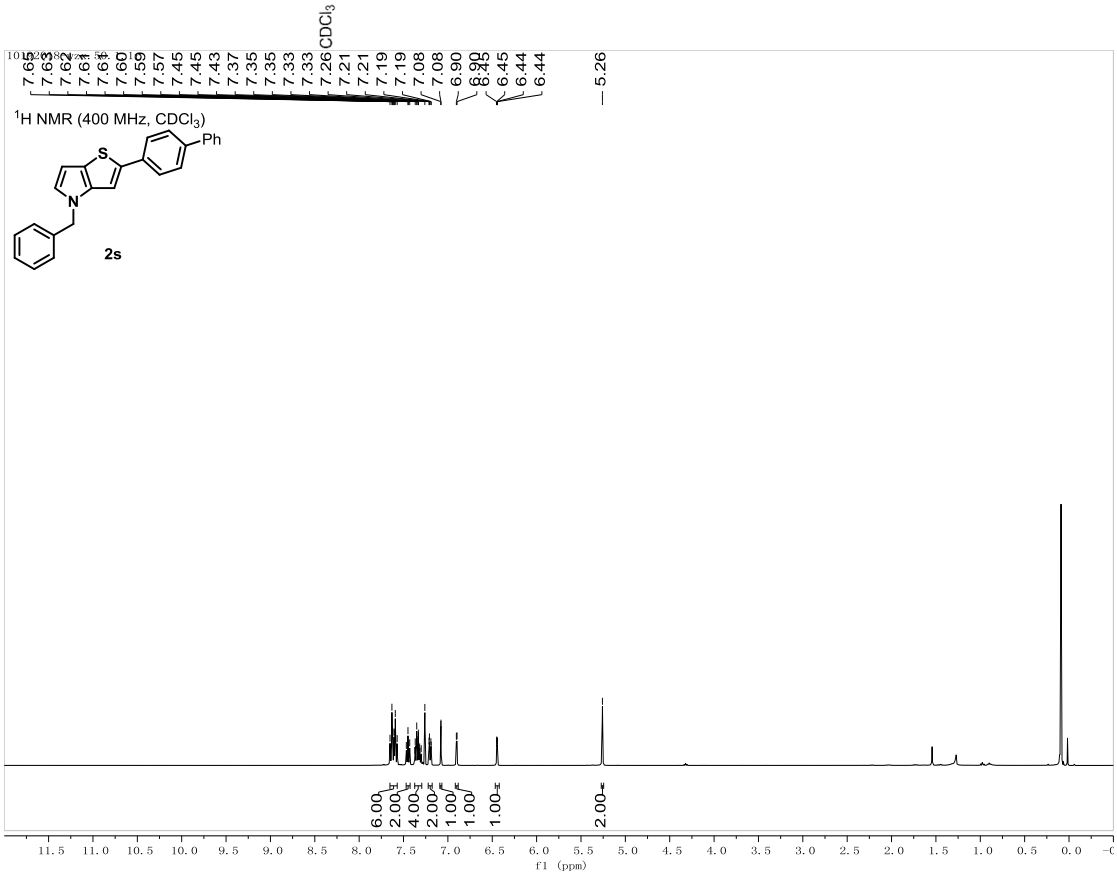

10132018-wzx. 30. 1. 1r
^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)
2q
139.8
139.1
137.3
135.2
128.9
127.9
127.7
127.0
126.2
123.6
122.9
107.2
101.1
77.4
77.1 CDCl$_3$
76.7
52.2
f1 (ppm)

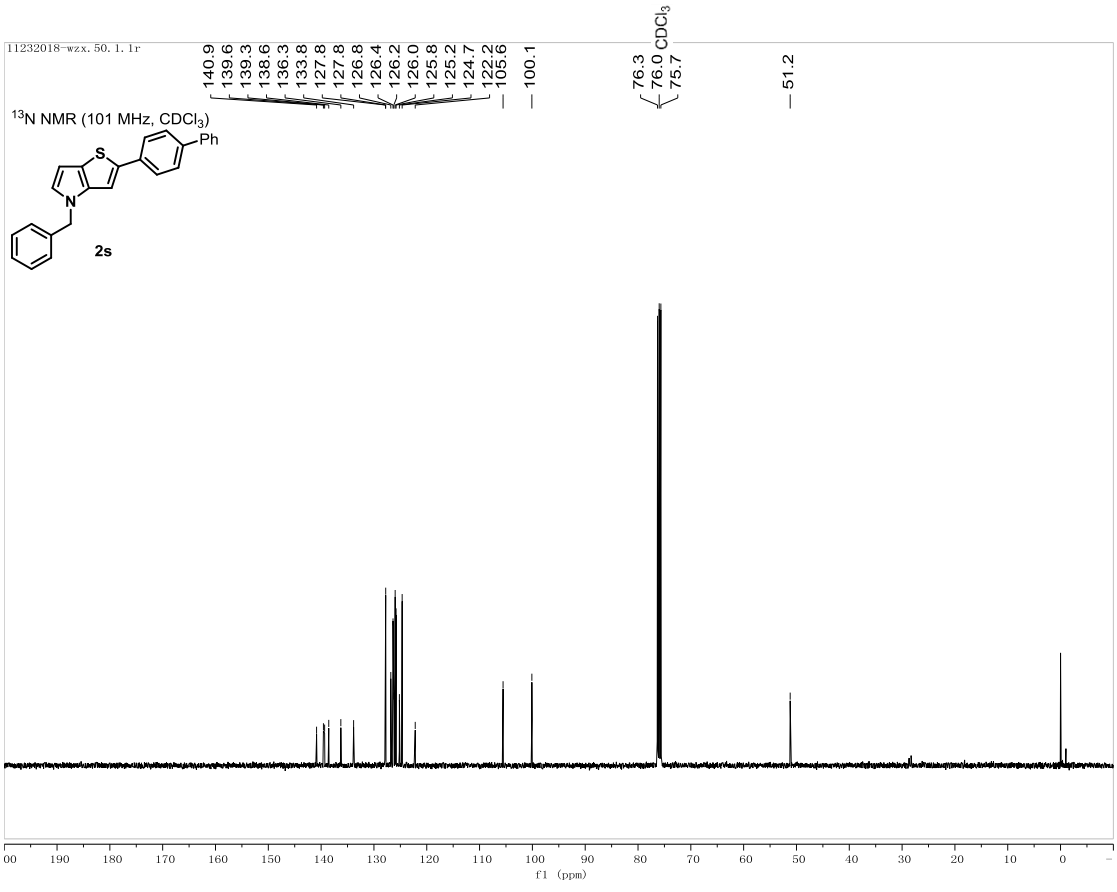


09292018-wzx.80.1.1r
7.32
7.32
7.31
7.31
7.30
7.29
7.29
7.28
7.28
7.26
CDCl3
7.25
7.24
7.24
7.23
7.16
7.15
7.15
7.14
7.13
6.87
6.85
6.84
6.39
6.38
5.20
1H NMR (400 MHz, CDCl3)
2r
4.02
2.00
2.00
1.00
1.00
1.00
2.00
f1 (ppm)

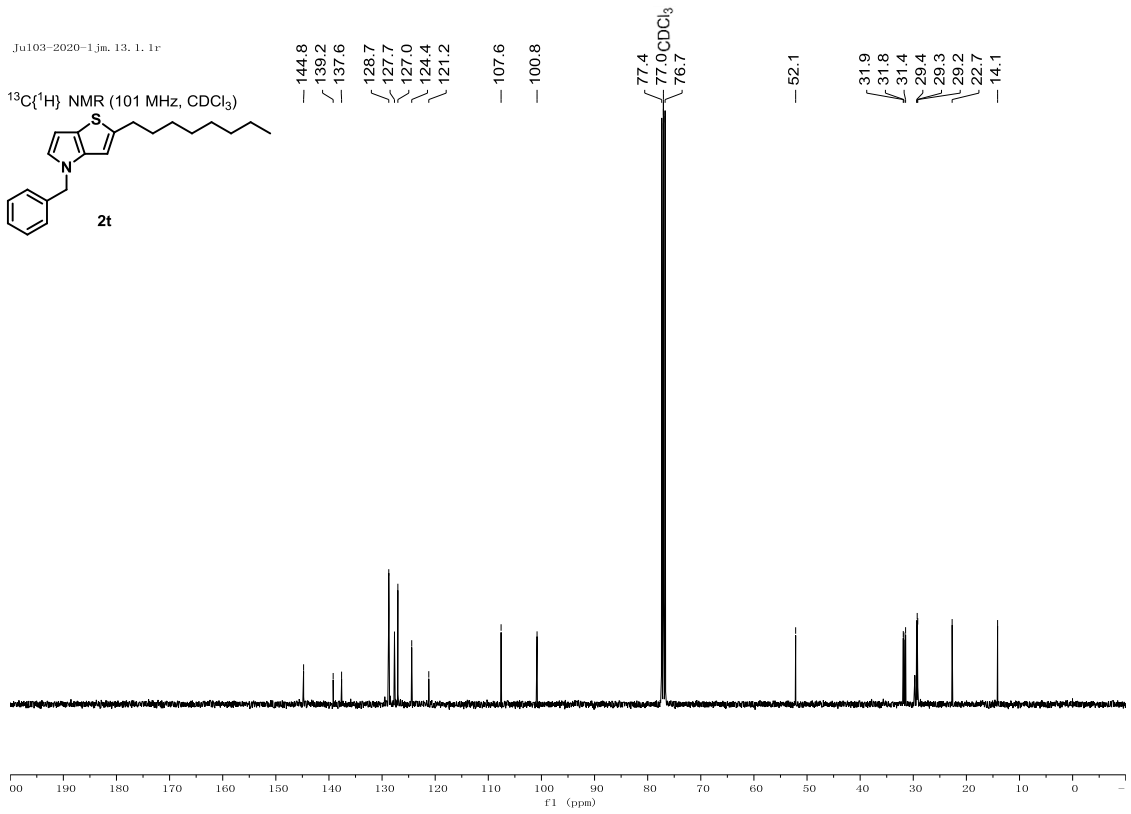


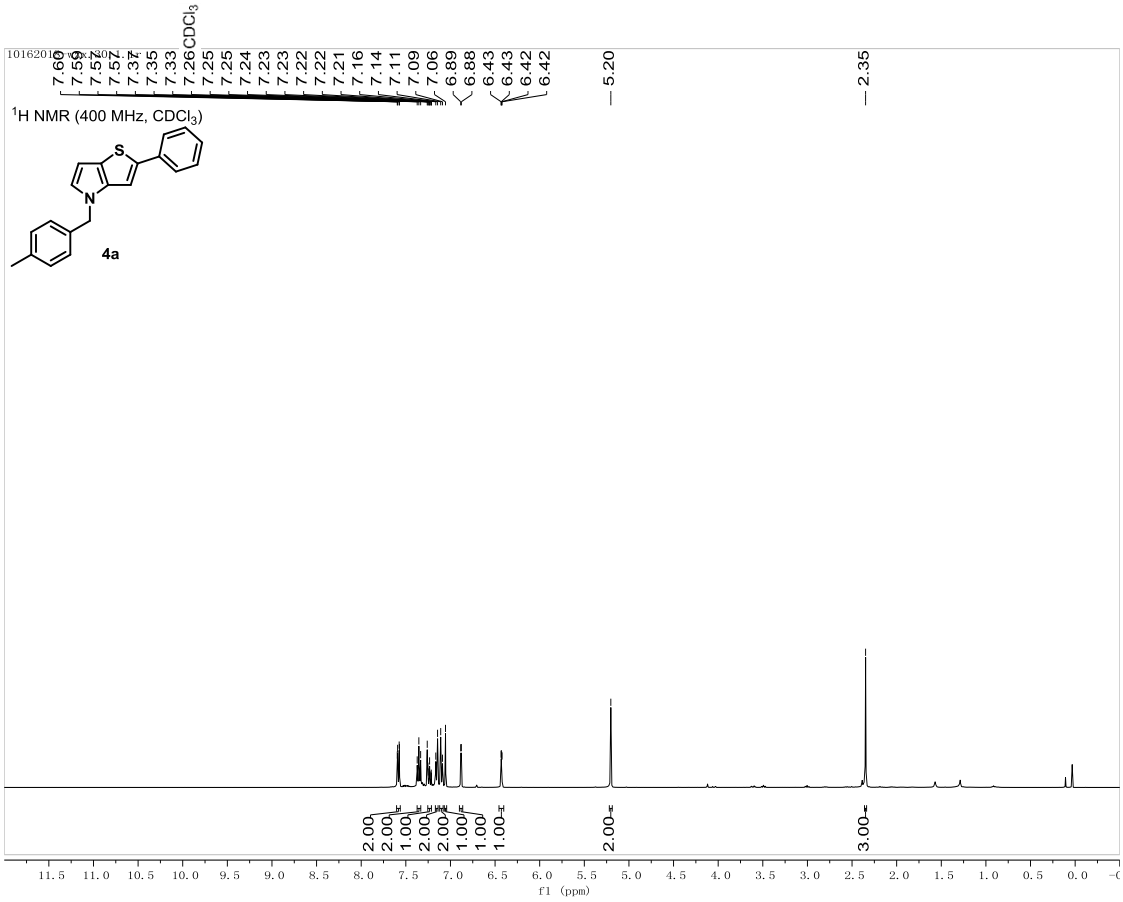
10152018-wzx.80.1.1r
13C{1H} NMR (101 MHz, CDCl3)
2r
139.9
137.3
137.2
137.1
128.8
127.8
127.0
126.0
126.0
125.9
122.3
118.4
106.7
101.0
77.3
77.0
CDCl3
76.7
52.2
f1 (ppm)

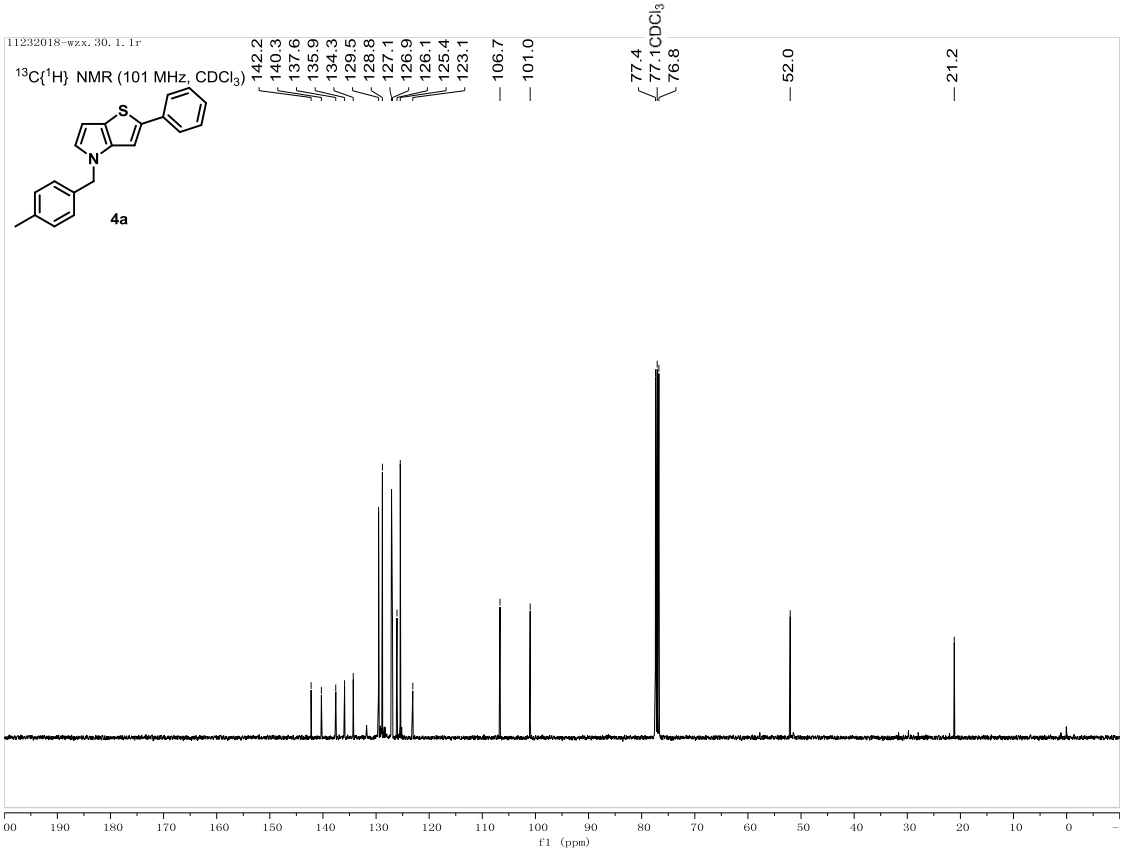

^{1}H NMR (400 MHz, $CDCl_3$)
Ph
S
N
2s
7.65
7.63
7.62
7.61
7.60
7.59
7.57
7.45
7.45
7.43
7.37
7.35
7.33
7.33
7.26 $CDCl_3$
7.21
7.21
7.19
7.19
7.08
7.08
6.90
6.90
6.45
6.44
6.44
5.26
6.00
2.00
4.00
2.00
1.00
1.00
1.00
2.00
f1 (ppm)

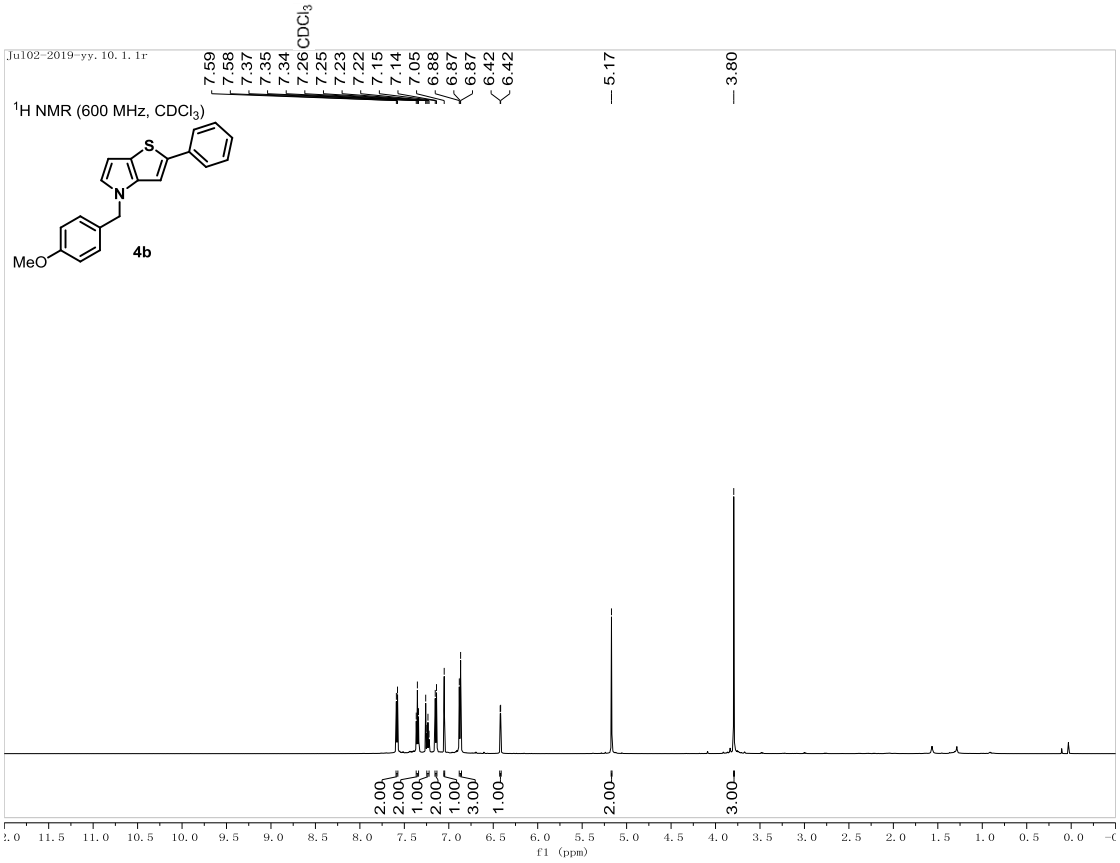

11232018-wzx. 50. 1. 1r
^{13}N NMR (101 MHz, $CDCl_3$)
Ph
S
N
2s
140.9
139.6
139.3
138.6
136.3
133.8
127.8
127.8
126.8
126.4
126.2
126.0
125.8
125.2
124.7
122.2
105.6
100.1
76.3
76.0 $CDCl_3$
75.7
51.2
f1 (ppm)

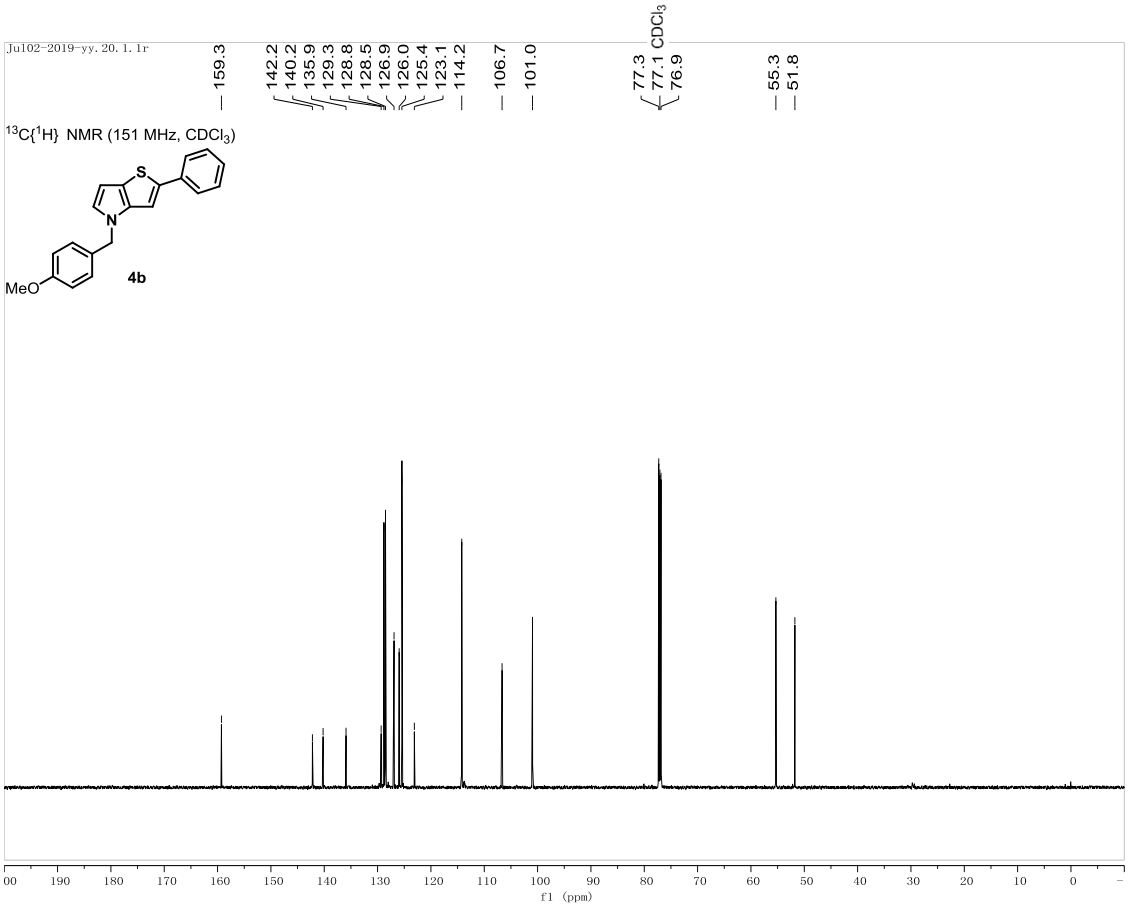
Ju103-2020-1jm. 10. 1. 1r
7.31
7.31
7.30
7.29
7.29
7.28
7.28
7.26CDCl3
7.25
7.16
7.15
7.14
7.14
7.13
6.78
6.77
6.49
6.35
6.34
5.16
2.79
2.77
2.75
2.75
1.67
1.65
1.63
1.61
1.29
1.29
1.27
1.26
1.25
1.24
1.23
0.89
0.89
0.88
0.87
0.86
0.86
1H NMR (400 MHz, CDCl3)
2t
4.00
2.00
1.00
1.00
1.00
1.02
2.00
2.00
10.00
3.00
f1 (ppm)

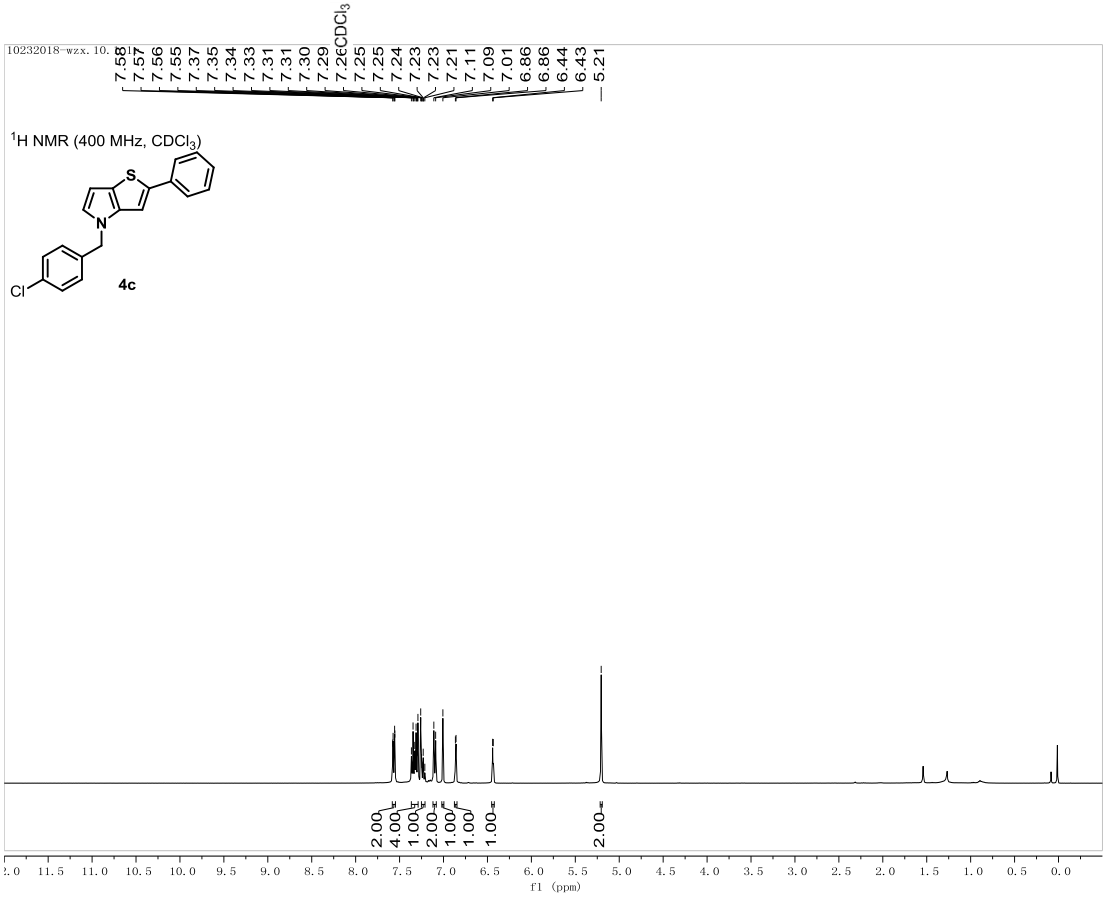

Ju103-2020-1jm. 13. 1. 1r
144.8
139.2
137.6
128.7
127.7
127.0
124.4
121.2
107.6
100.8
77.4
77.0CDCl3
76.7
52.1
31.9
31.8
31.4
29.4
29.3
29.2
22.7
14.1
13C{1H} NMR (101 MHz, CDCl3)
2t
f1 (ppm)

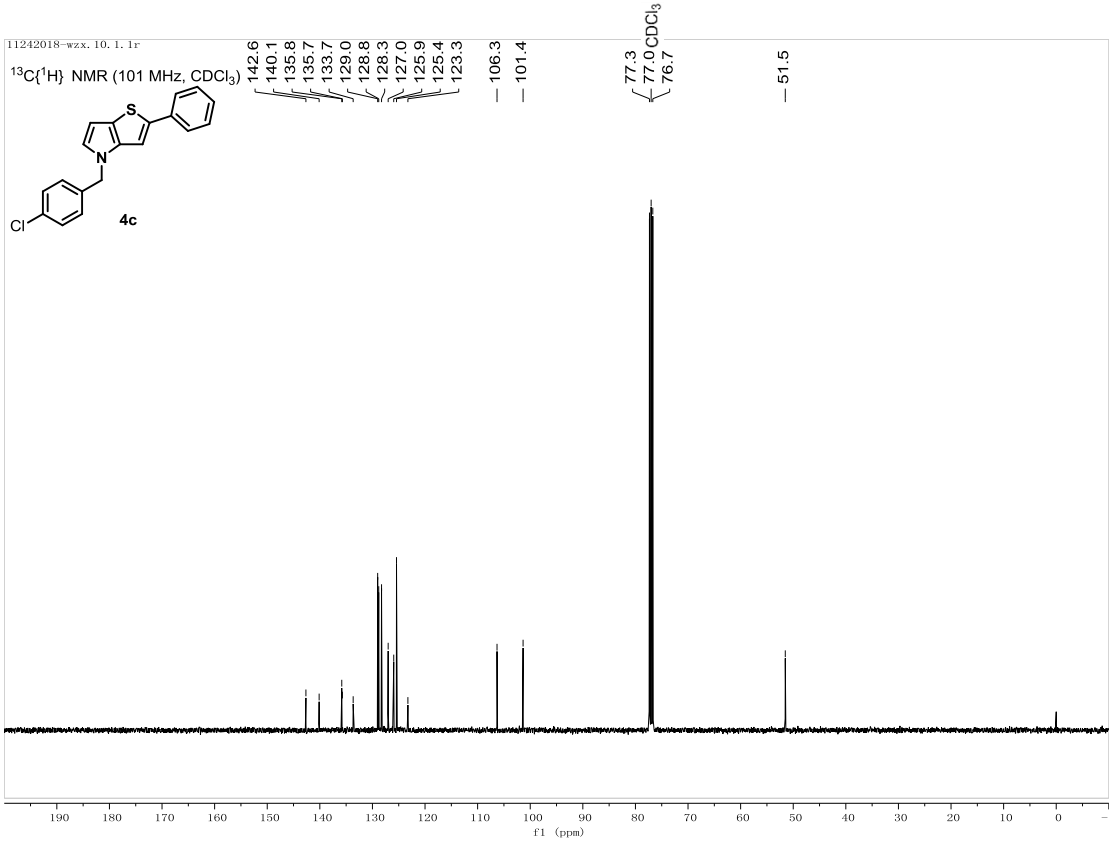

^{1}H NMR (400 MHz, $CDCl_3$)
4a
7.60
7.59
7.57
7.57
7.37
7.35
7.33
7.26 $CDCl_3$
7.25
7.25
7.24
7.23
7.23
7.22
7.22
7.21
7.16
7.14
7.11
7.09
7.06
6.89
6.88
6.43
6.43
6.42
6.42
5.20
2.35
2.00
2.00
1.00
2.00
2.00
1.00
1.00
2.00
3.00
f1 (ppm)

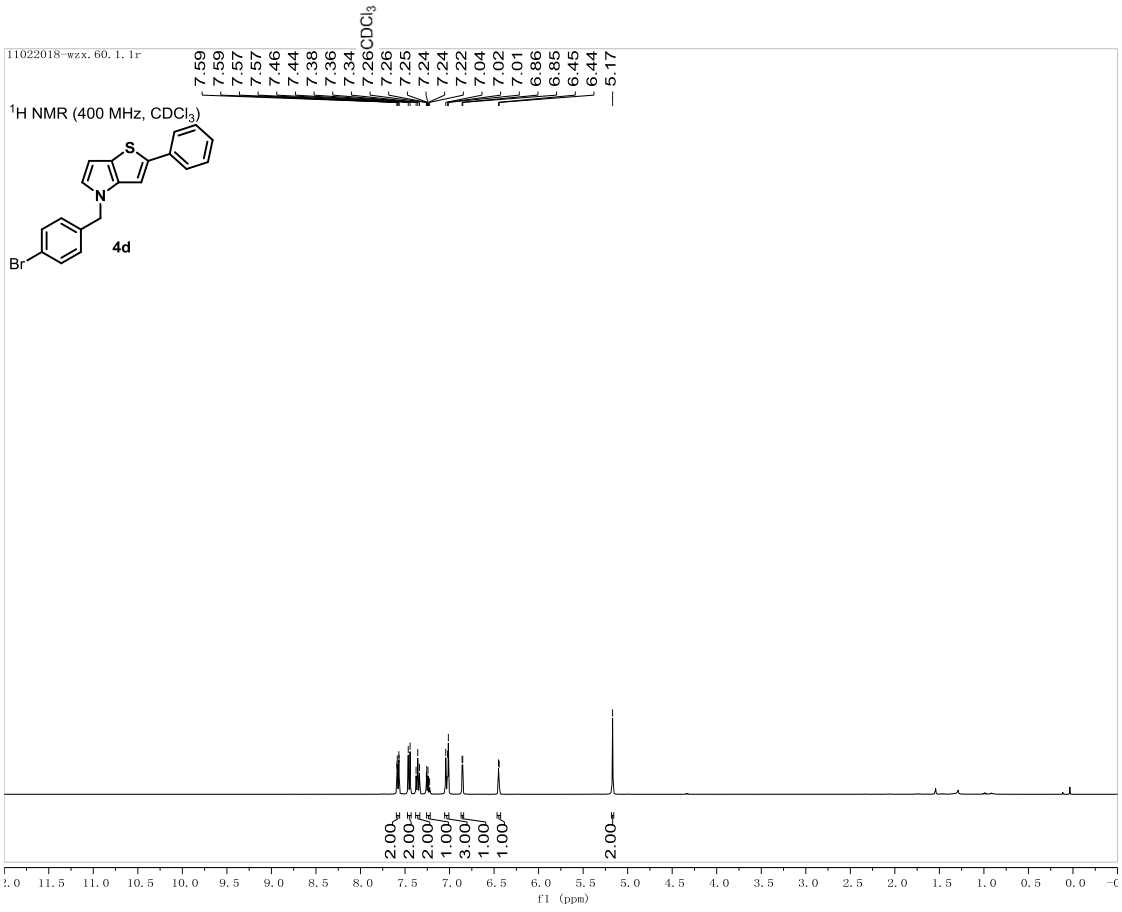

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)
4a
142.2
140.3
137.6
135.9
134.3
129.5
128.8
127.1
126.9
126.1
125.4
123.1
106.7
101.0
77.4
77.1 $CDCl_3$
76.8
52.0
21.2
f1 (ppm)

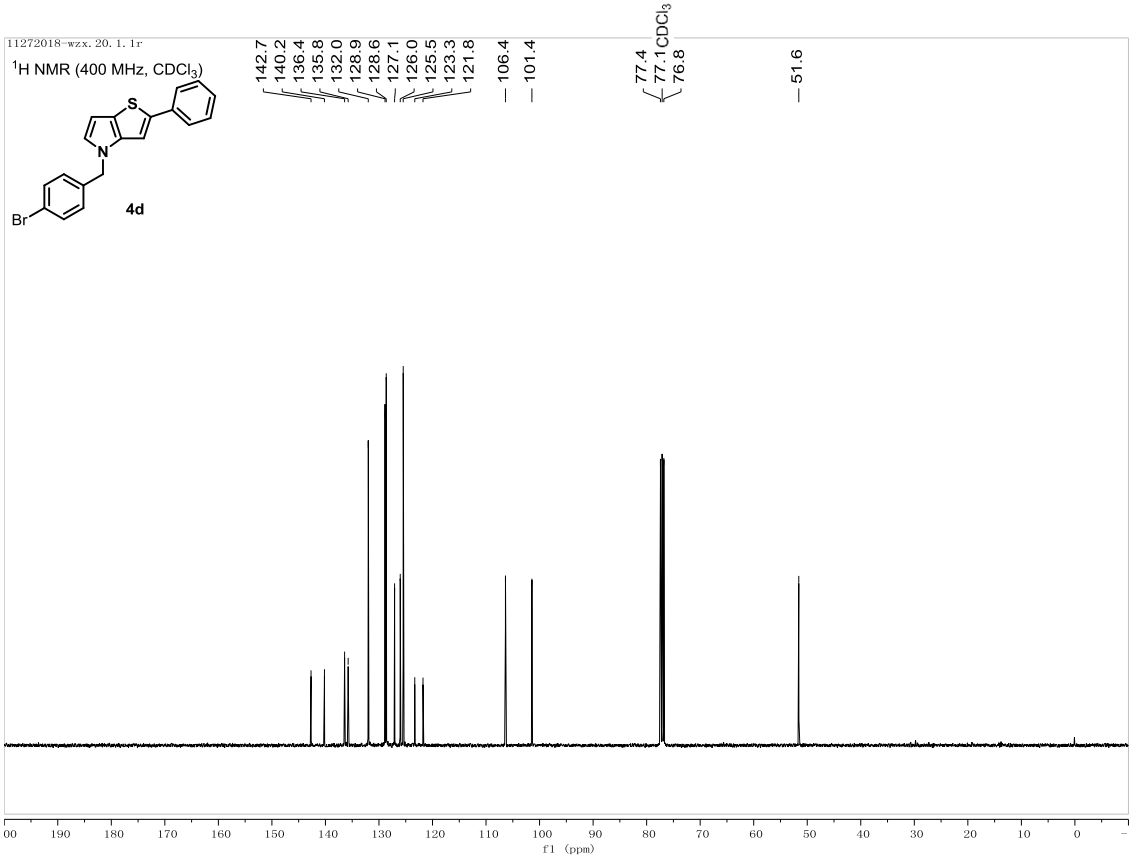

Ju102-2019-yy. 10. 1. 1r
7.59
7.58
7.37
7.35
7.34
7.26 CDCl3
7.25
7.23
7.22
7.15
7.14
7.05
6.88
6.87
6.87
6.42
6.42
5.17
3.80
1H NMR (600 MHz, CDCl3)
S
N
MeO
4b
2.00
2.00
1.00
2.00
1.00
3.00
1.00
2.00
3.00
f1 (ppm)

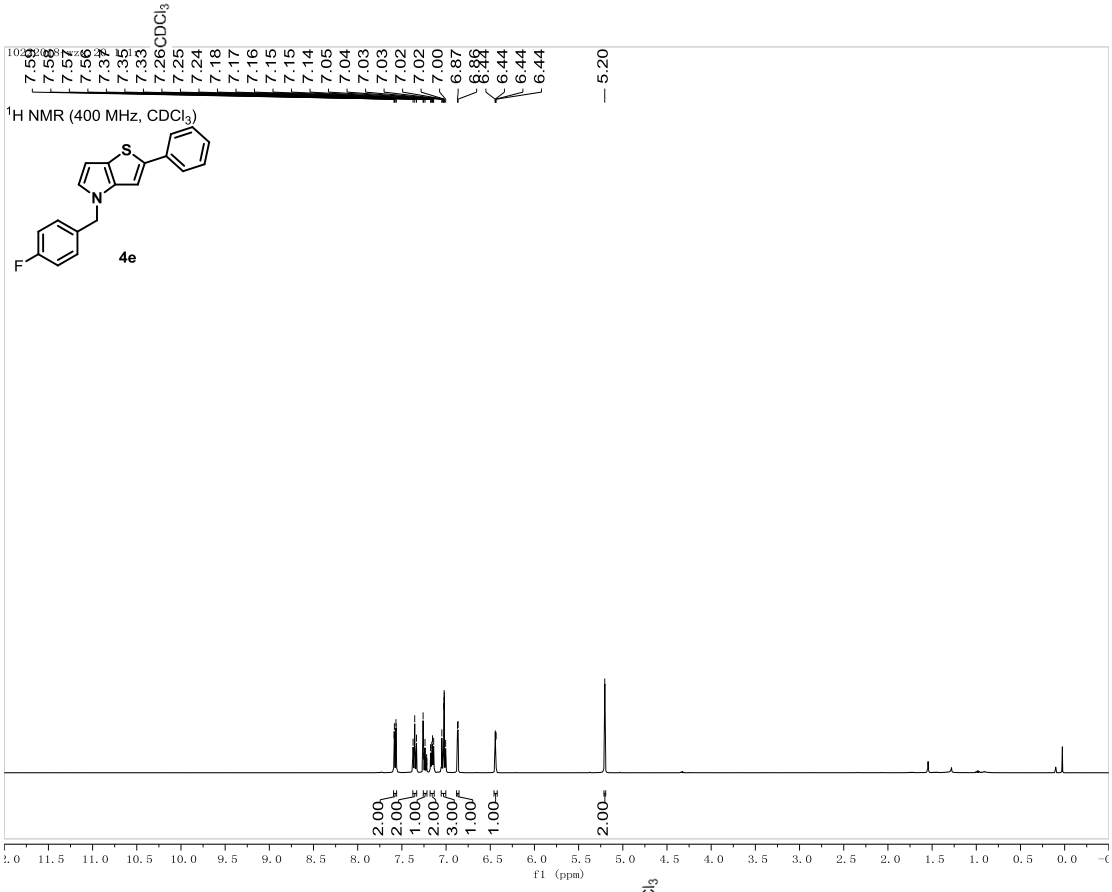

Ju102-2019-yy. 20. 1. 1r
159.3
142.2
140.2
135.9
129.3
128.8
128.5
126.9
126.0
125.4
123.1
114.2
106.7
101.0
77.3
77.1 CDCl3
76.9
55.3
51.8
13C{1H} NMR (151 MHz, CDCl3)
S
N
MeO
4b
f1 (ppm)

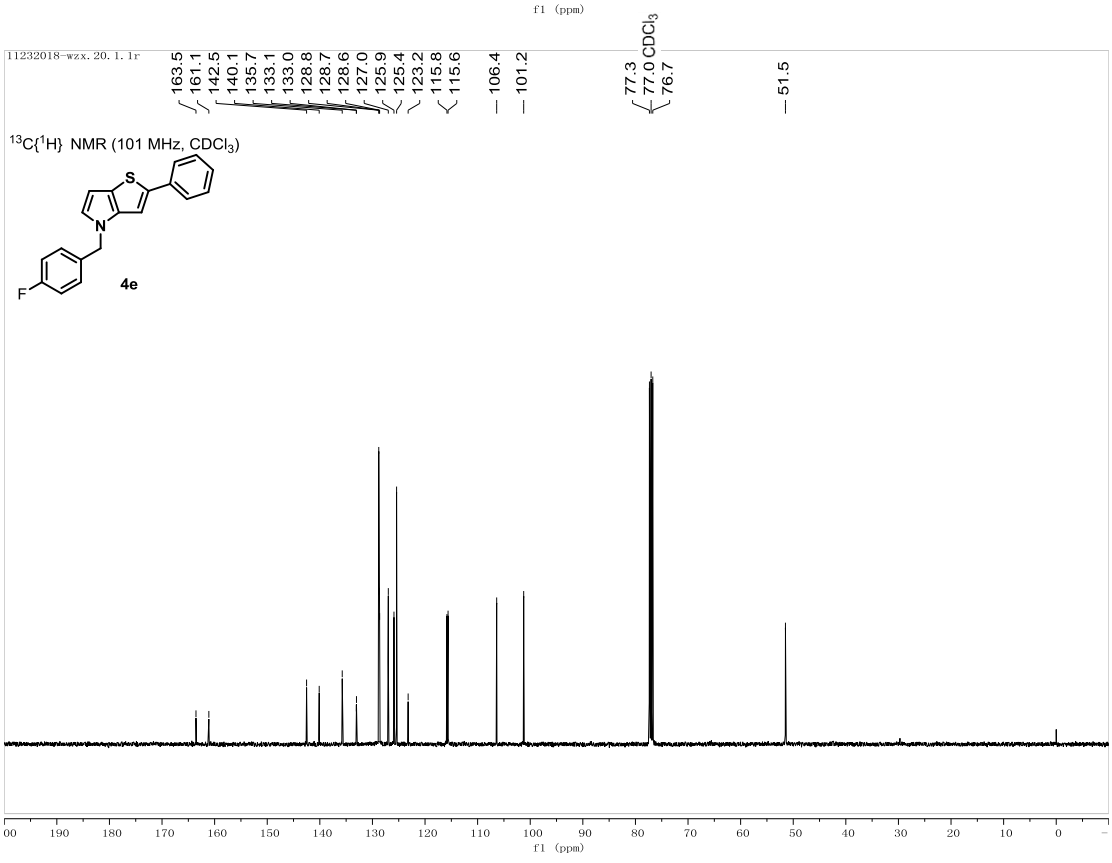

10232018-wzx. 10.
7.58
7.57
7.56
7.55
7.37
7.35
7.34
7.33
7.31
7.31
7.30
7.29
7.26CDCl3
7.25
7.25
7.24
7.23
7.23
7.21
7.11
7.09
7.01
6.86
6.86
6.44
6.43
5.21
1H NMR (400 MHz, CDCl3)
S
N
Cl
4c
2.00
4.00
1.00
2.00
1.00
1.00
2.00
f1 (ppm)

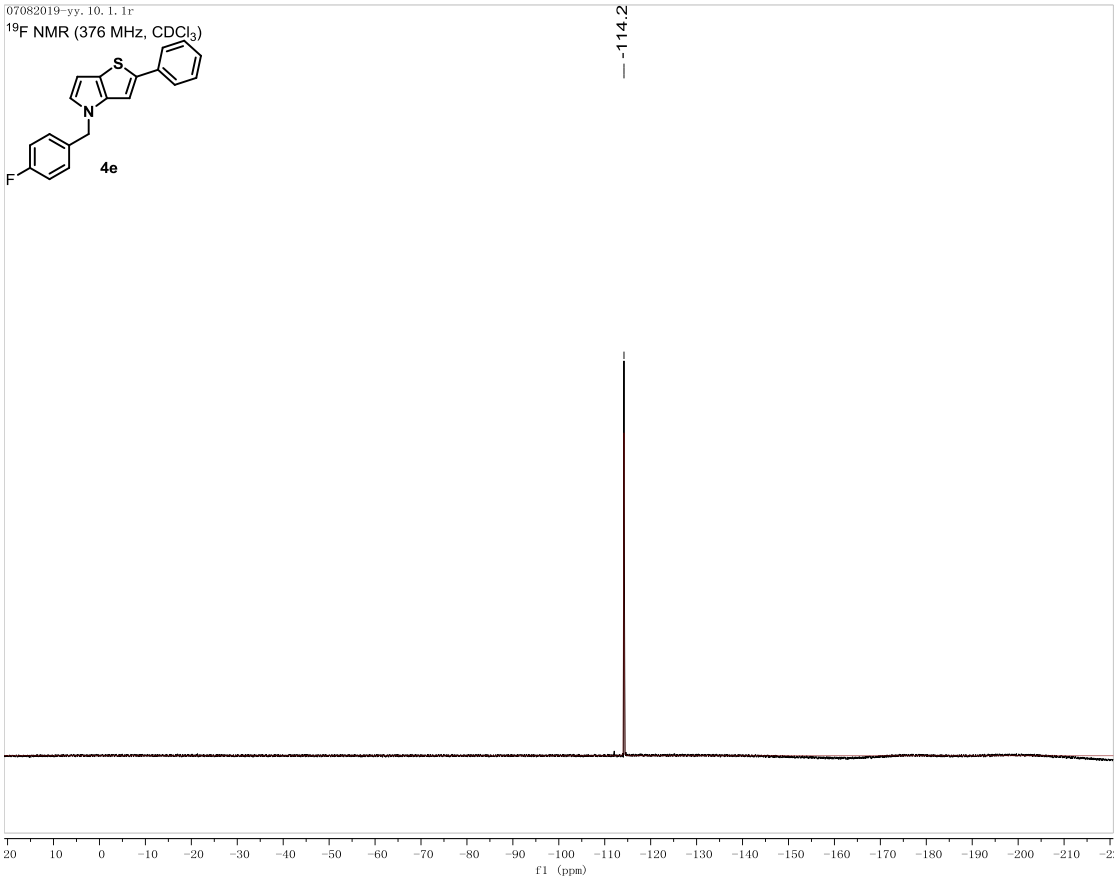

11242018-wzx. 10. 1. 1r
13C{1H} NMR (101 MHz, CDCl3)
142.6
140.1
135.8
135.7
133.7
129.0
128.8
128.3
127.0
125.9
125.4
123.3
106.3
101.4
77.3
77.0CDCl3
76.7
51.5
S
N
Cl
4c
f1 (ppm)

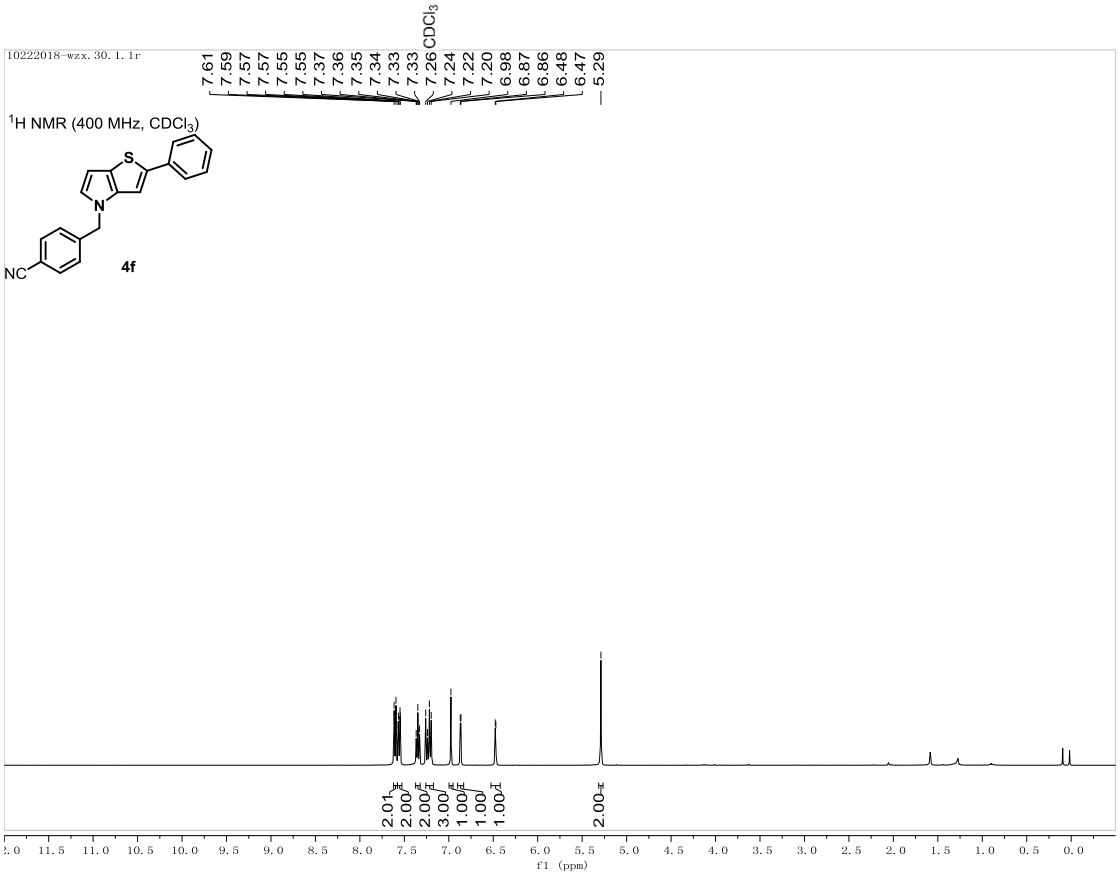

11022018-wzx. 60. 1. 1r
7.59
7.59
7.57
7.57
7.46
7.44
7.38
7.36
7.34
7.26CDCl3
7.26
7.25
7.24
7.24
7.22
7.04
7.02
7.01
6.86
6.85
6.45
6.44
5.17
1H NMR (400 MHz, CDCl3)
S
N
Br
4d
2.00
2.00
2.00
1.00
3.00
1.00
1.00
2.00
f1 (ppm)

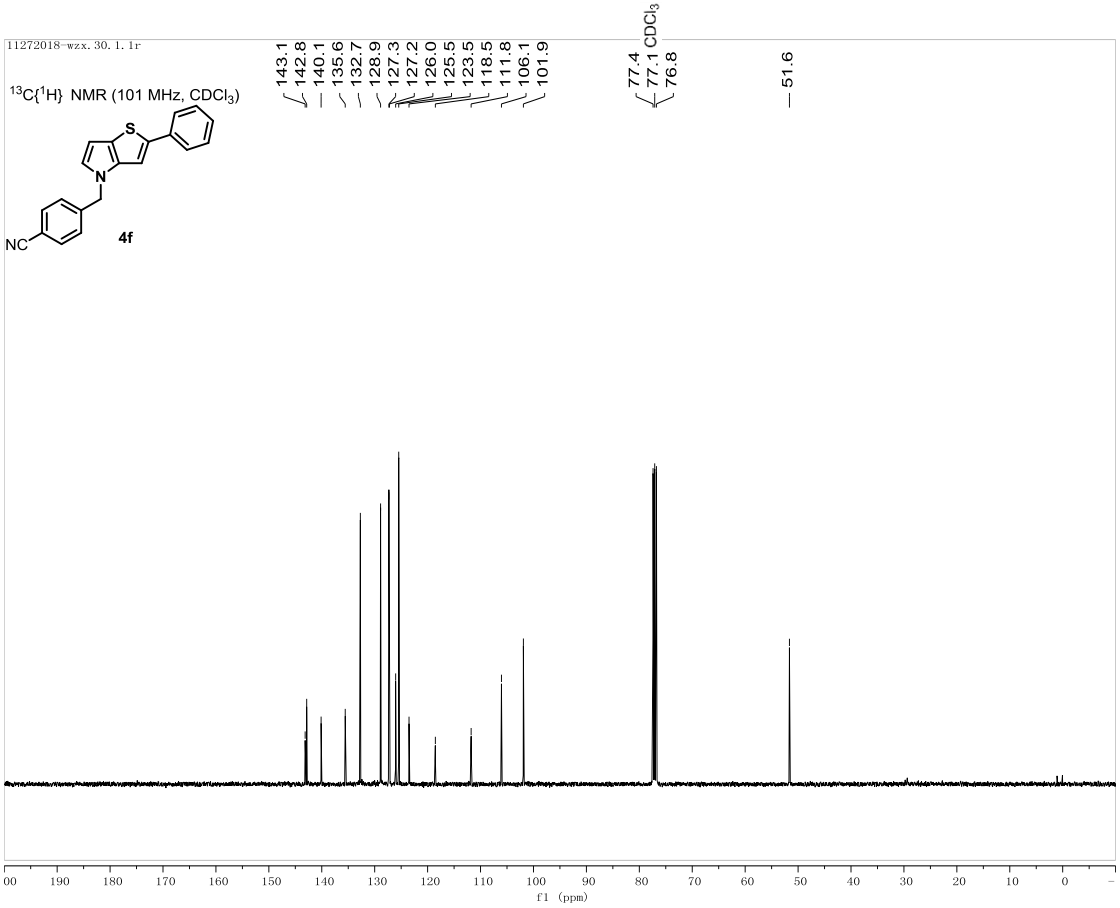

11272018-wzx. 20. 1. 1r
142.7
140.2
136.4
135.8
132.0
128.9
128.6
127.1
126.0
125.5
123.3
121.8
106.4
101.4
77.4
77.1CDCl3
76.8
51.6
1H NMR (400 MHz, CDCl3)
S
N
Br
4d
f1 (ppm)

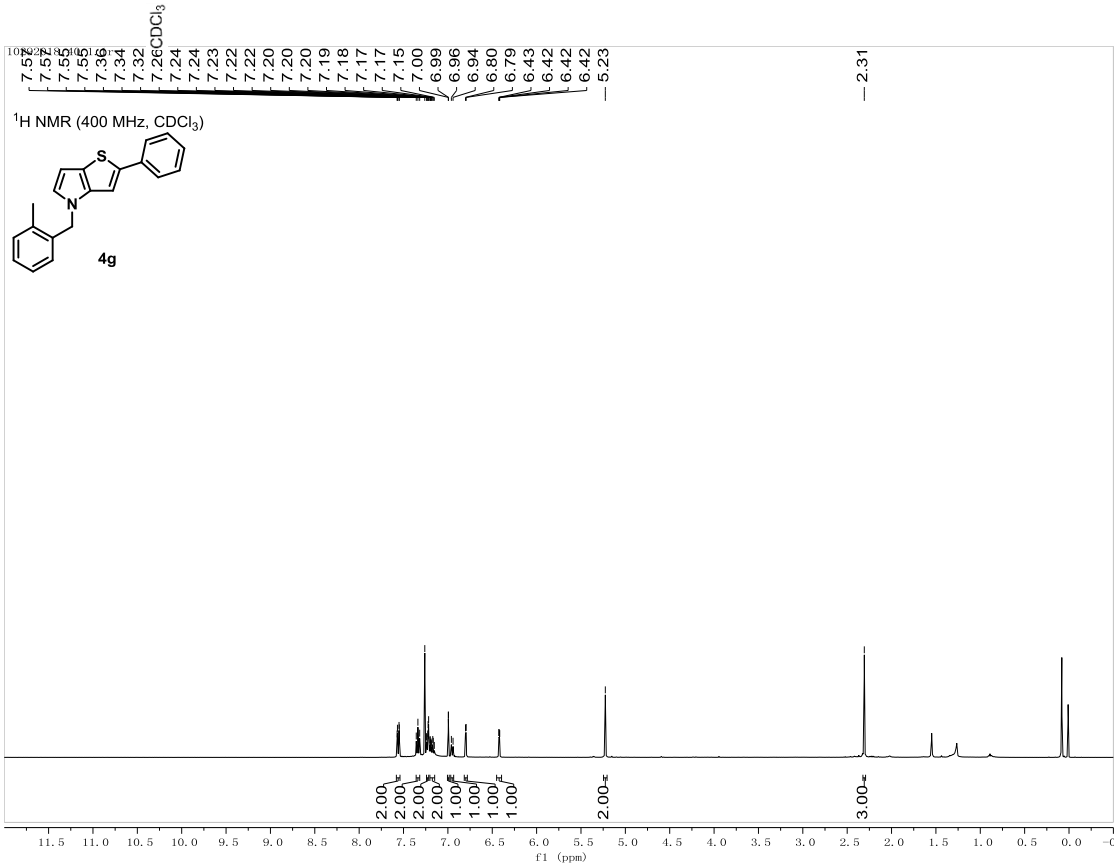

7.59
7.58
7.57
7.56
7.37
7.35
7.33
7.26CDCl3
7.25
7.24
7.18
7.17
7.16
7.15
7.15
7.14
7.05
7.04
7.03
7.03
7.02
7.02
7.00
6.87
6.86
6.44
6.44
6.44
6.44
5.20
1H NMR (400 MHz, CDCl3)
S
N
F
4e
2.00
2.00
1.00
2.00
3.00
1.00
1.00
2.00
f1 (ppm)

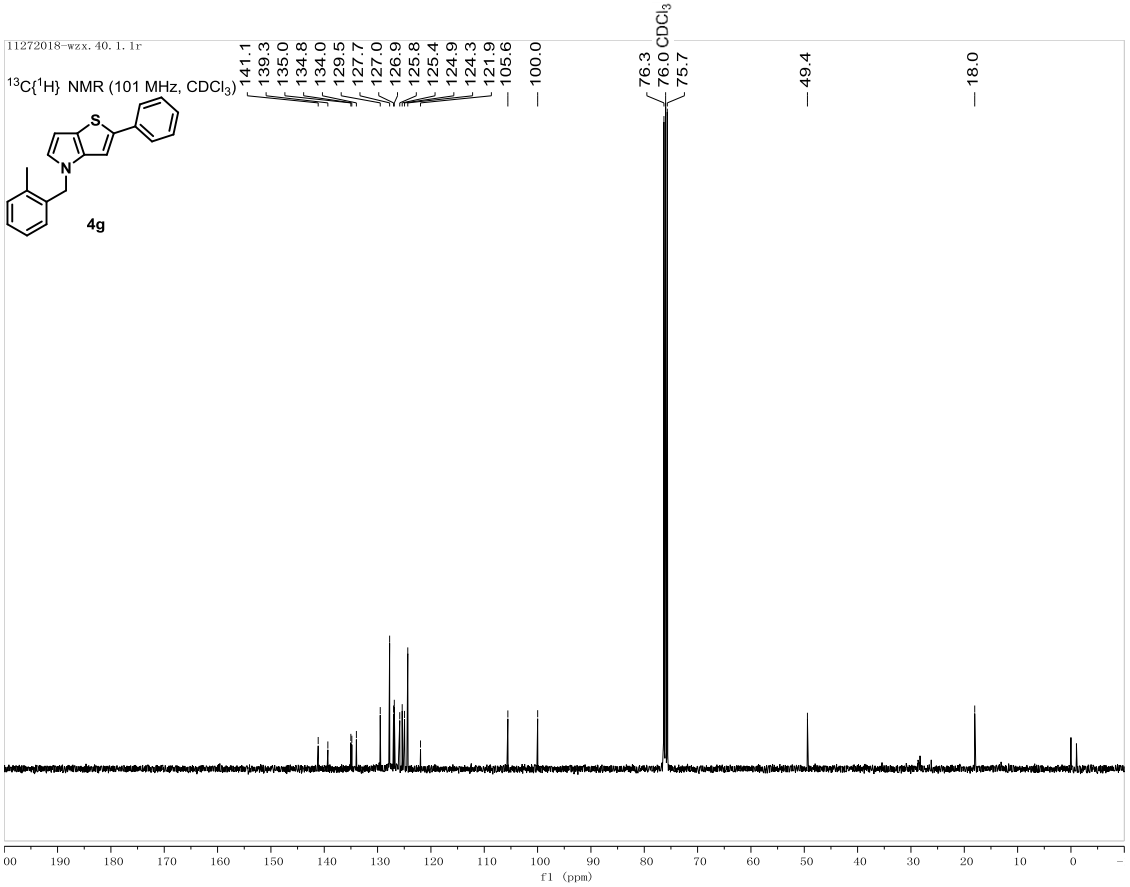

11232018-wzx. 20. 1. 1r
163.5
161.1
142.5
140.1
135.7
133.1
133.0
128.8
128.7
128.6
127.0
125.9
125.4
123.2
115.8
115.6
106.4
101.2
77.3
77.0 CDCl3
76.7
51.5
13C{1H} NMR (101 MHz, CDCl3)
S
N
F
4e
f1 (ppm)

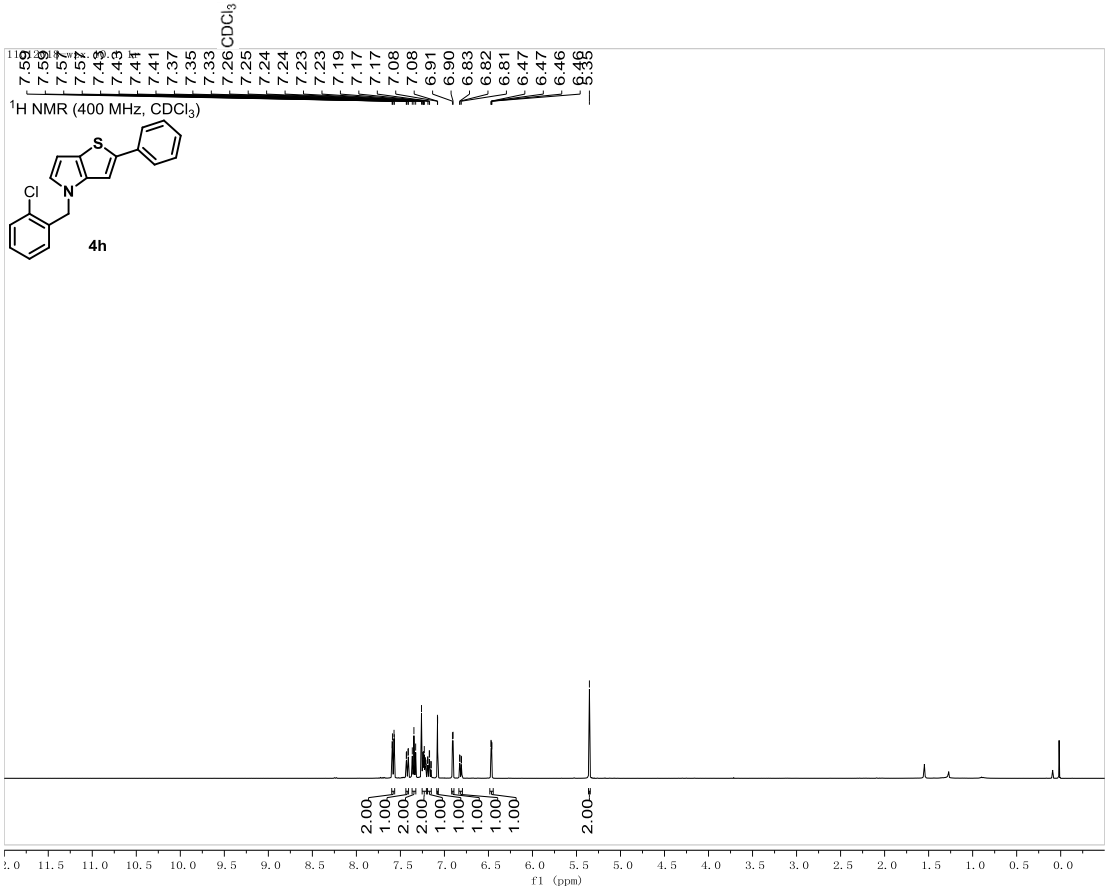

07082019-yy. 10. 1. 1r
19F NMR (376 MHz, CDCl3)
S
N
F
4e
-114.2
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

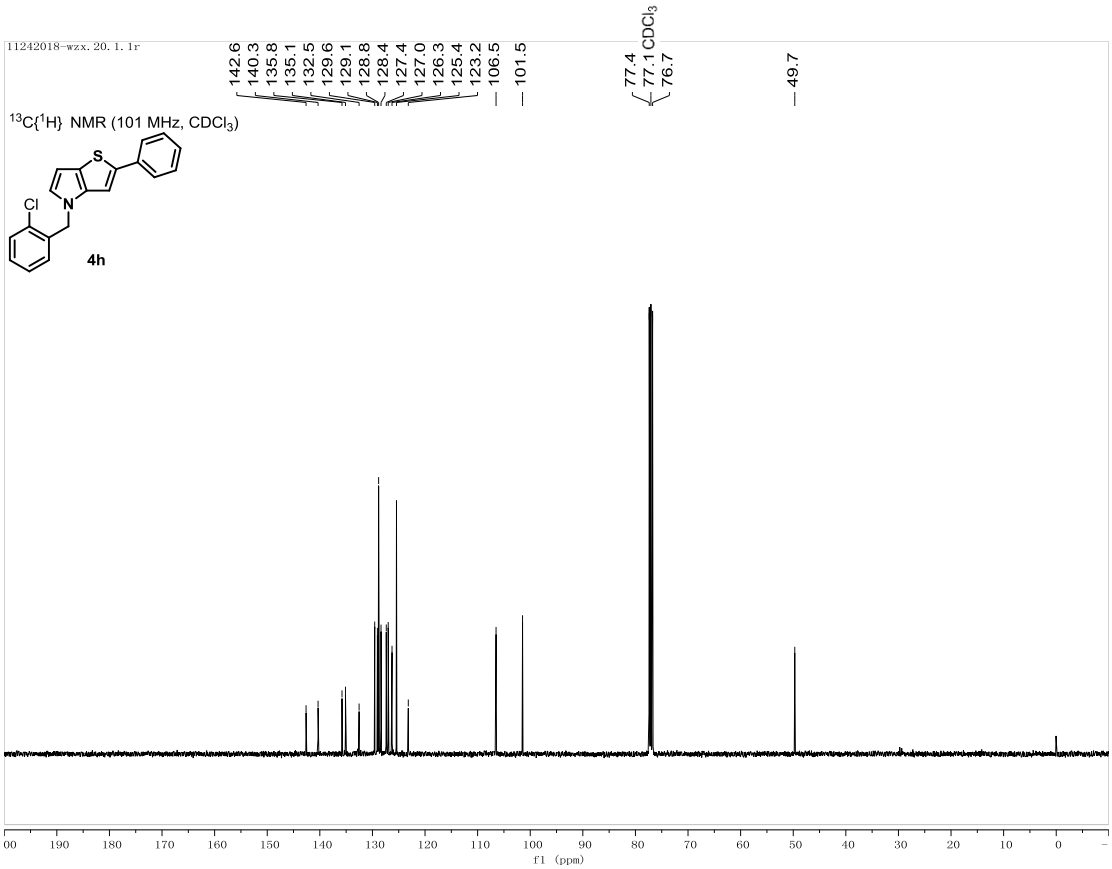

10222018-wzx. 30. 1. 1r
^{1}H NMR (400 MHz, CDCl$_3$)
4f
7.61
7.59
7.57
7.57
7.55
7.55
7.37
7.36
7.35
7.34
7.33
7.33
7.26 CDCl$_3$
7.24
7.22
7.20
6.98
6.87
6.86
6.48
6.47
5.29
2.01
2.00
2.00
3.00
1.00
1.00
1.00
2.00
f1 (ppm)

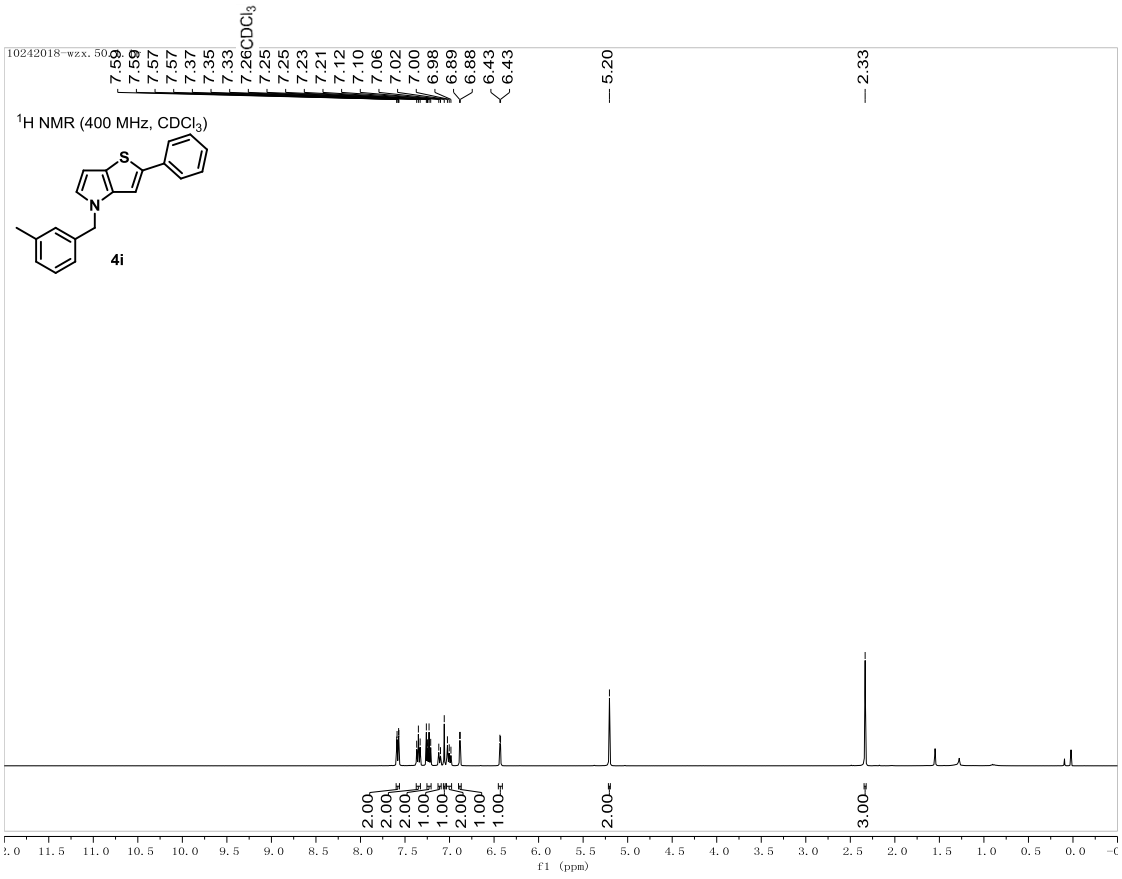

11272018-wzx. 30. 1. 1r
^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)
4f
143.1
142.8
140.1
135.6
132.7
128.9
127.3
127.2
126.0
125.5
123.5
118.5
111.8
106.1
101.9
77.4
77.1 CDCl$_3$
76.8
51.6
f1 (ppm)

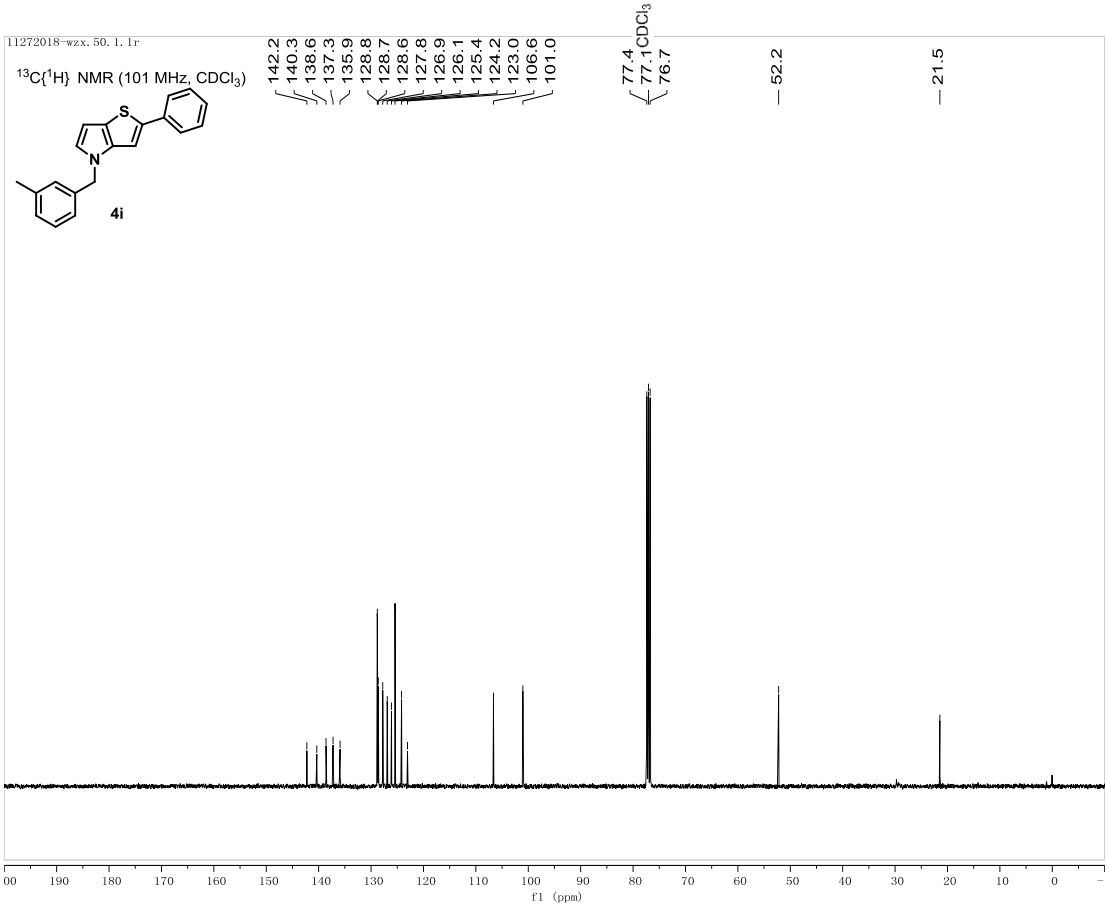

^{1}H NMR (400 MHz, CDCl$_3$)
4g
7.57
7.56
7.55
7.55
7.36
7.34
7.32
7.26 CDCl$_3$
7.24
7.24
7.23
7.22
7.22
7.20
7.20
7.20
7.19
7.18
7.17
7.17
7.15
7.00
6.99
6.96
6.94
6.80
6.79
6.43
6.42
6.42
6.42
5.23
2.31
2.00
2.00
2.00
2.00
1.00
1.00
1.00
2.00
3.00
f1 (ppm)

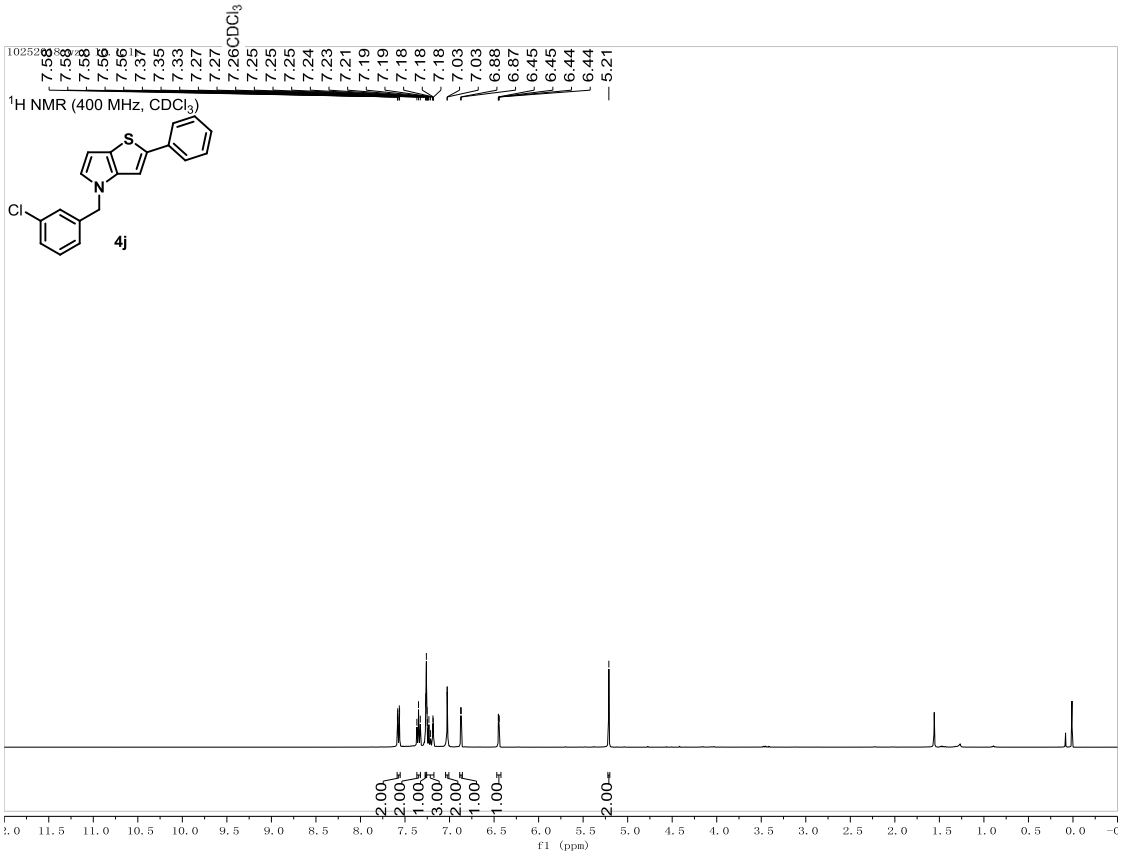

11272018-wzx. 40. 1. 1r
^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)
4g
141.1
139.3
135.0
134.8
134.0
129.5
127.7
127.0
126.9
125.8
125.4
124.9
124.3
121.9
105.6
100.0
76.3
76.0 CDCl$_3$
75.7
49.4
18.0
f1 (ppm)

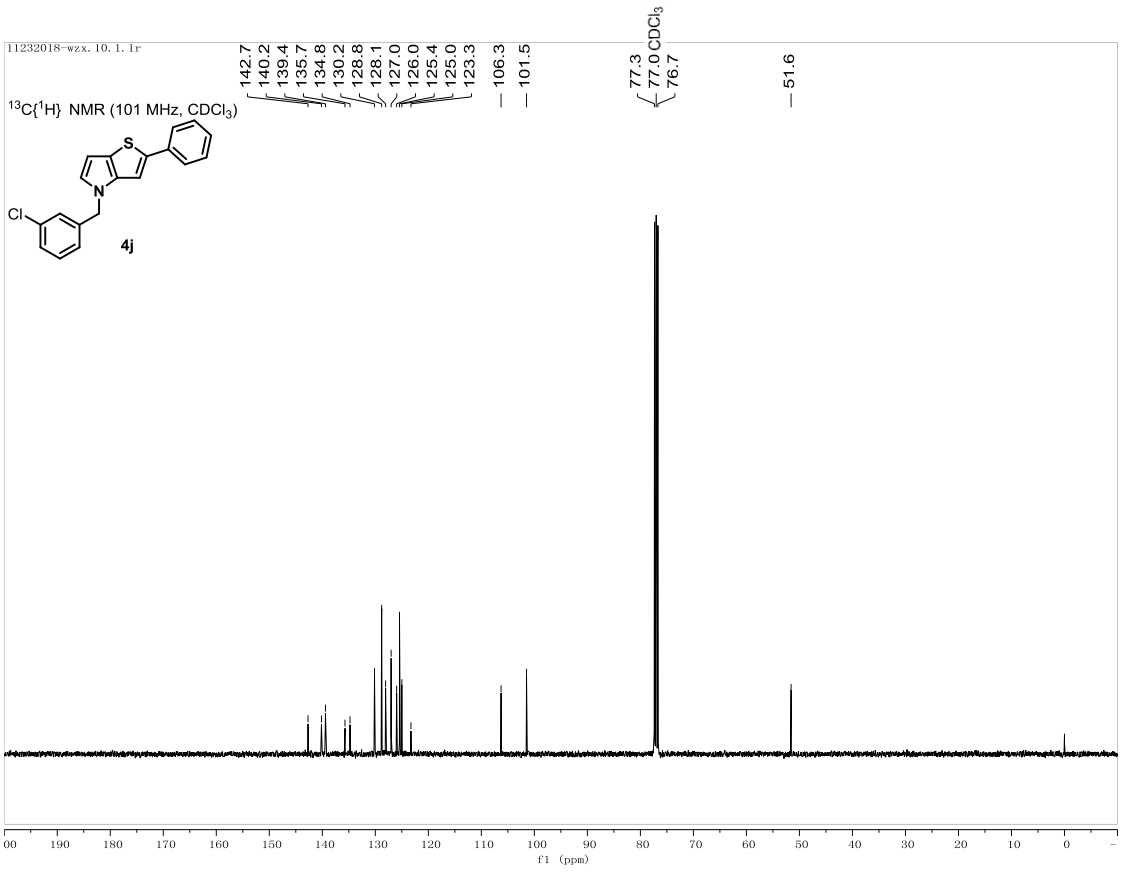

^{1}H NMR (400 MHz, CDCl$_3$)
4h

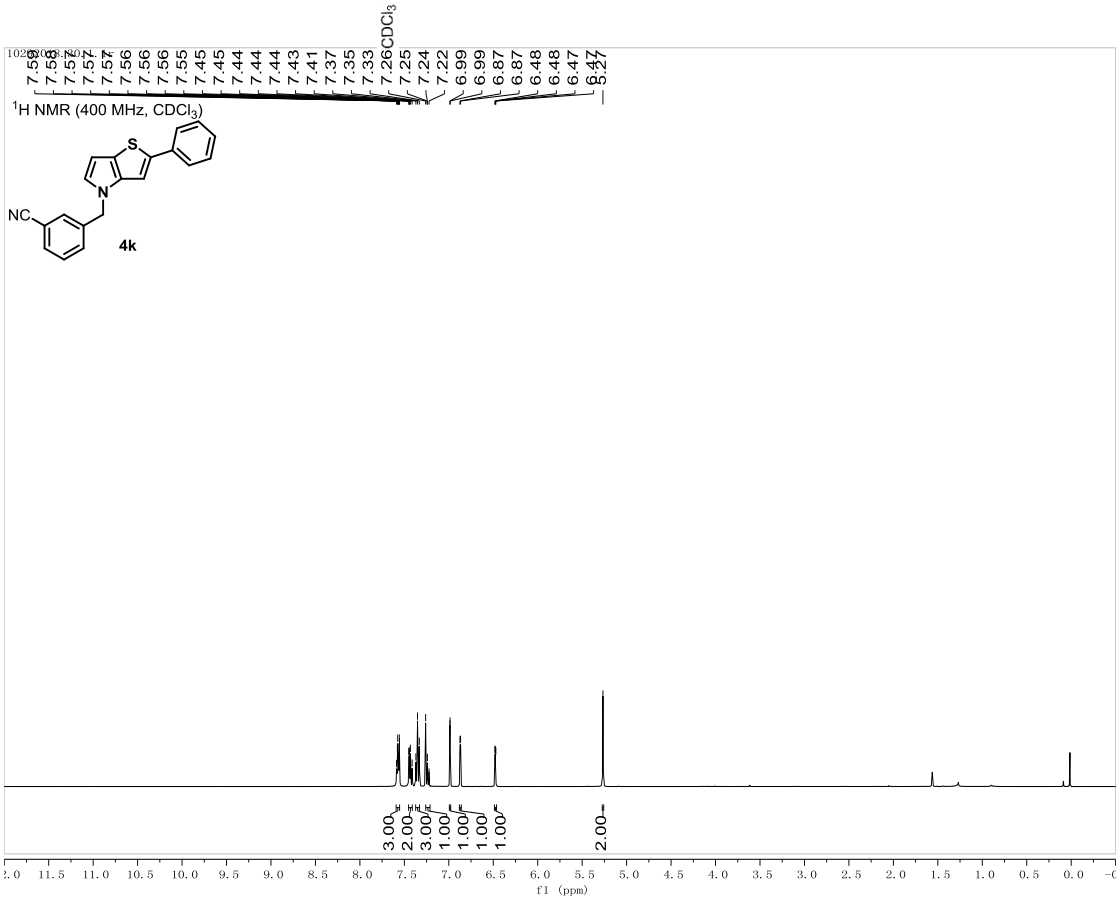

^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)
4h

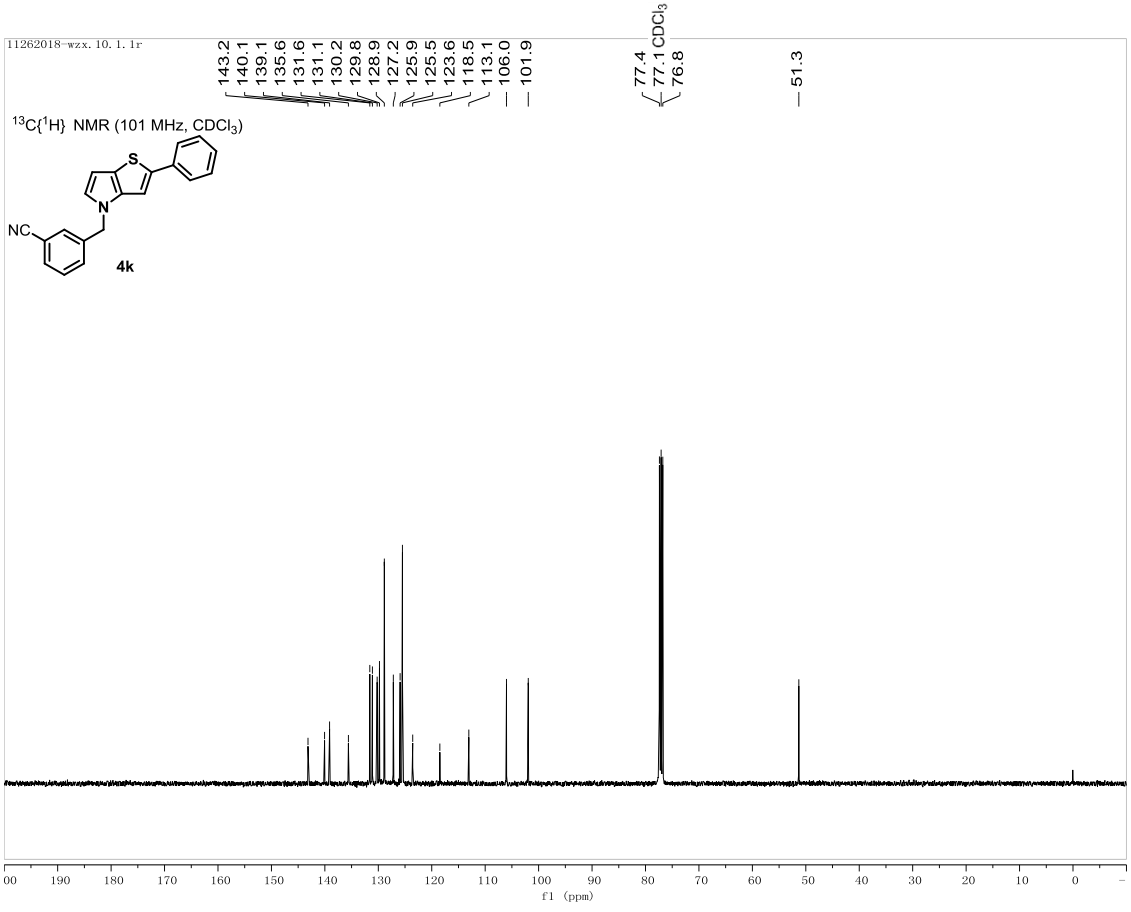

10242018-wzx. 50.1
7.59
7.59
7.57
7.57
7.37
7.35
7.33
7.26CDCl3
7.25
7.25
7.23
7.21
7.12
7.10
7.06
7.02
7.00
6.98
6.89
6.88
6.43
6.43
5.20
2.33
1H NMR (400 MHz, CDCl3)
4i
2.00
2.00
1.00
1.00
2.00
1.00
1.00
2.00
3.00
f1 (ppm)

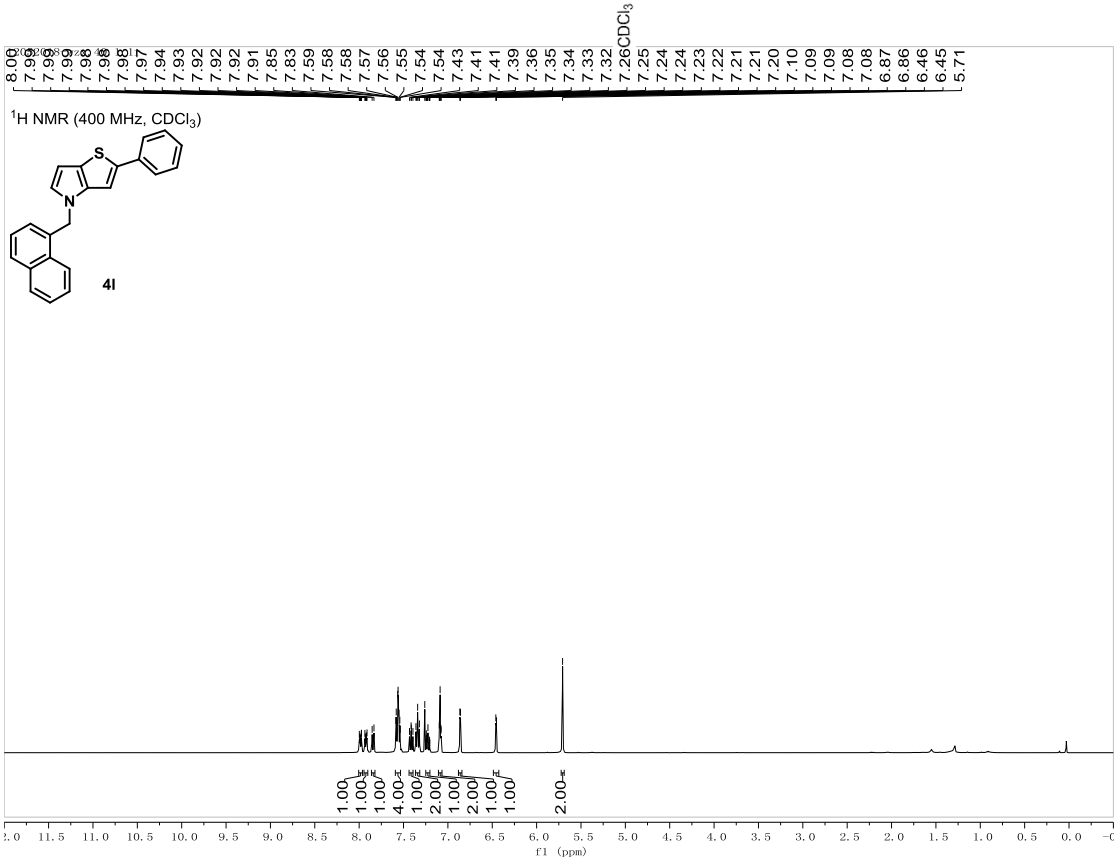

11272018-wzx. 50. 1. 1r
13C{1H} NMR (101 MHz, CDCl3)
4i
142.2
140.3
138.6
137.3
135.9
128.8
128.7
128.6
127.8
126.9
126.1
125.4
124.2
123.0
106.6
101.0
77.4
77.1CDCl3
76.7
52.2
21.5
f1 (ppm)

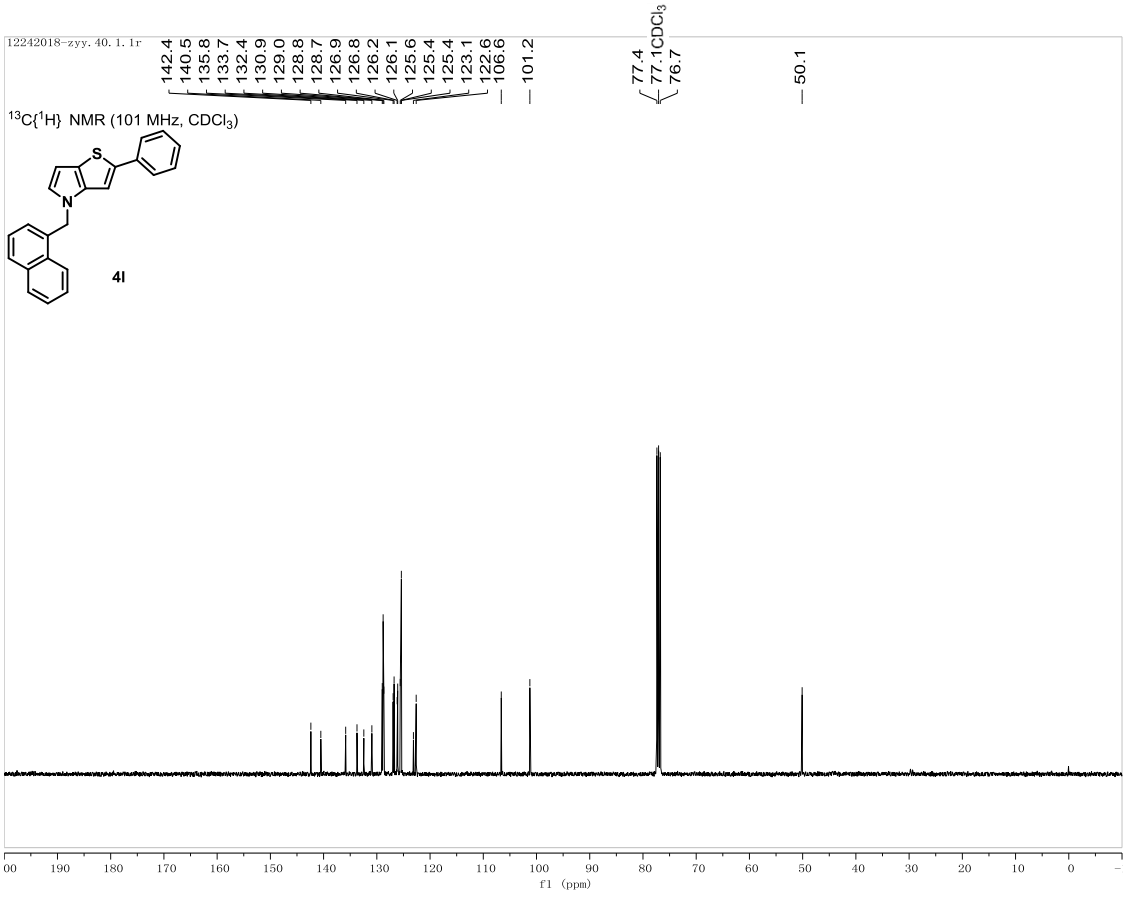

^{1}H NMR (400 MHz, CDCl$_3$)
4j
f1 (ppm)

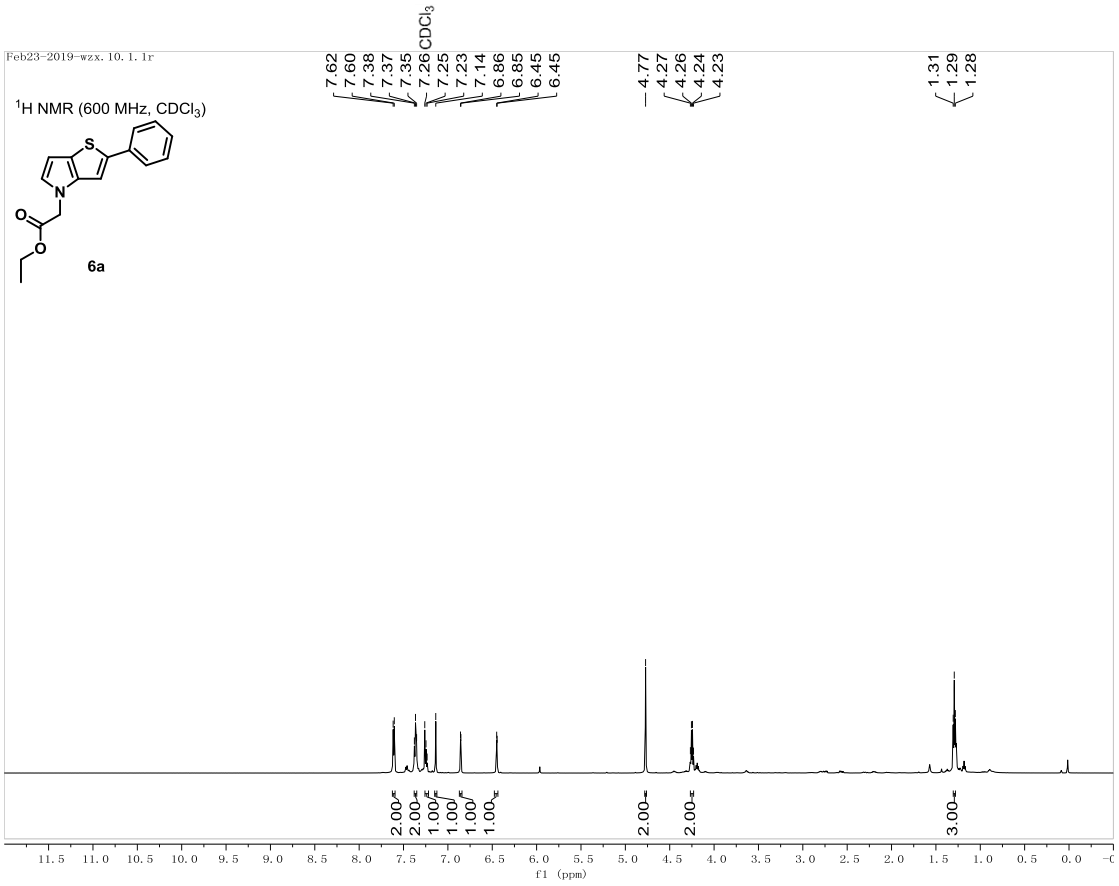

^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)
4j
f1 (ppm)

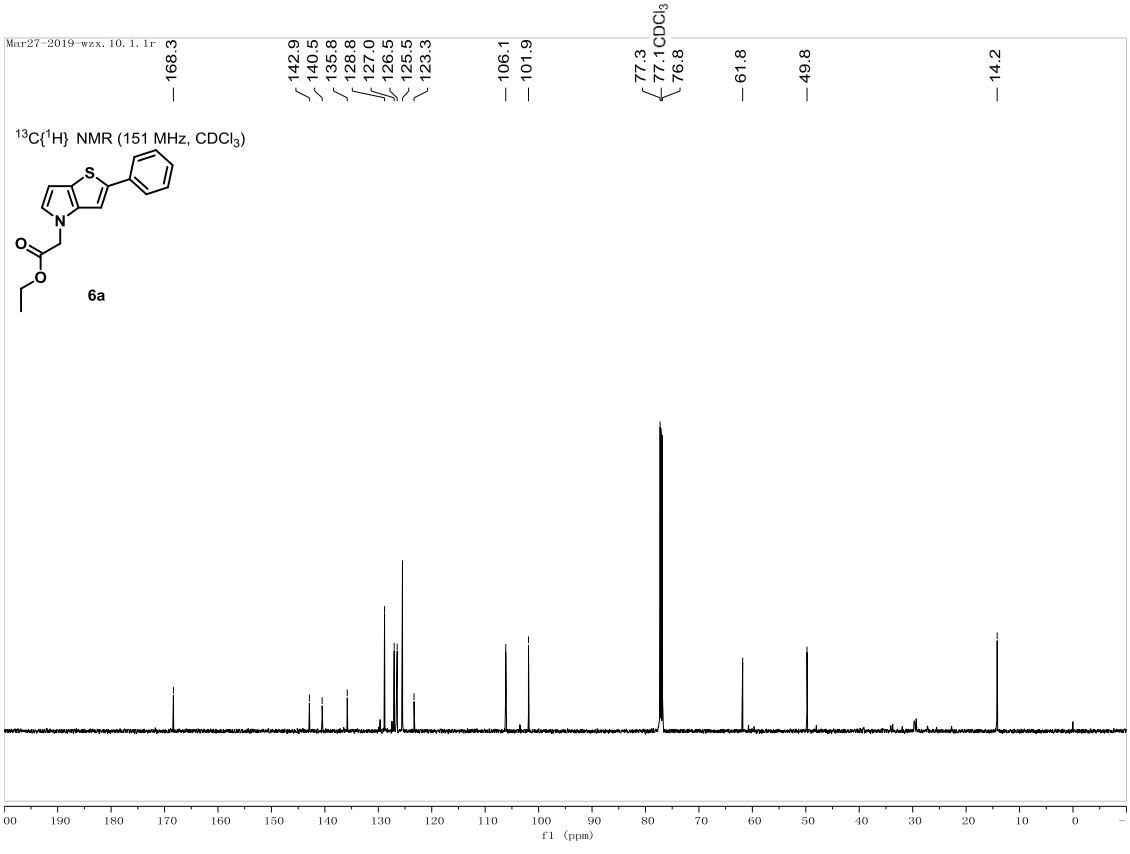

1H NMR (400 MHz, CDCl3)
4k
f1 (ppm)

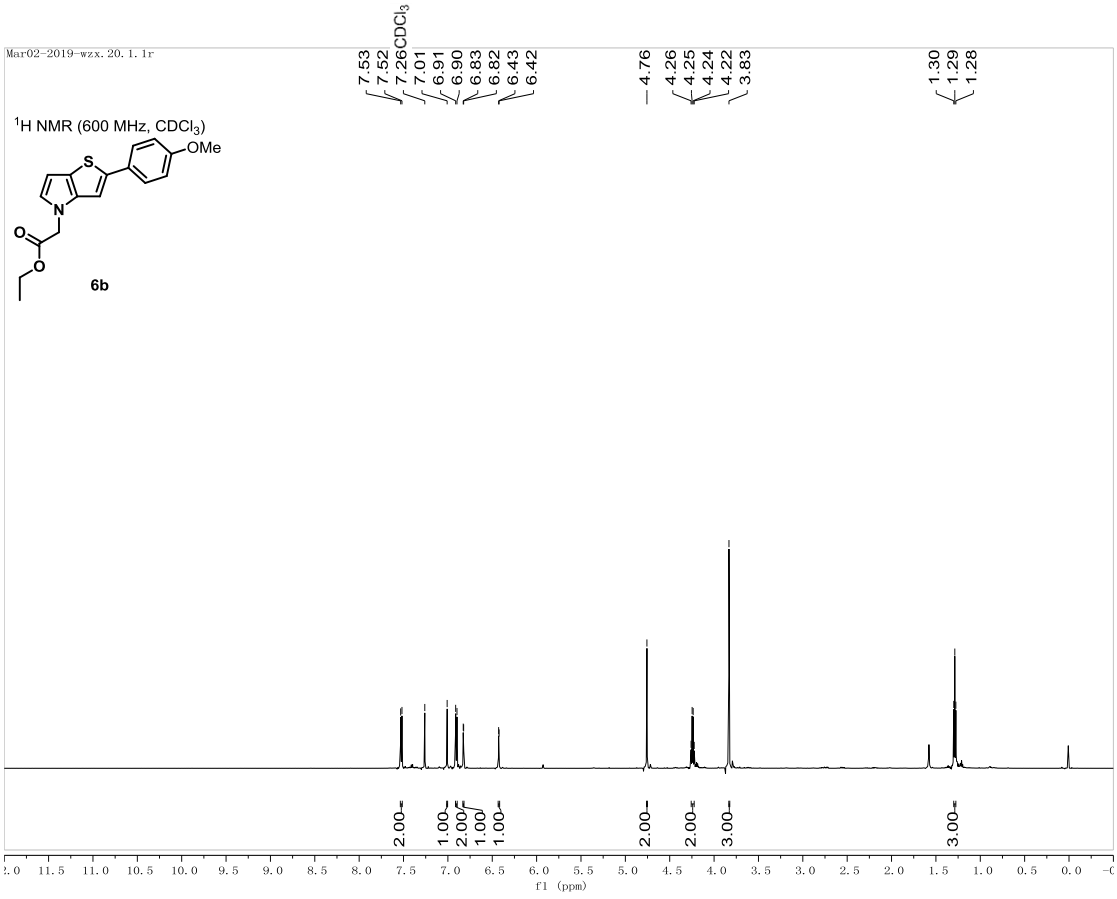

13C{1H} NMR (101 MHz, CDCl3)
4k
f1 (ppm)

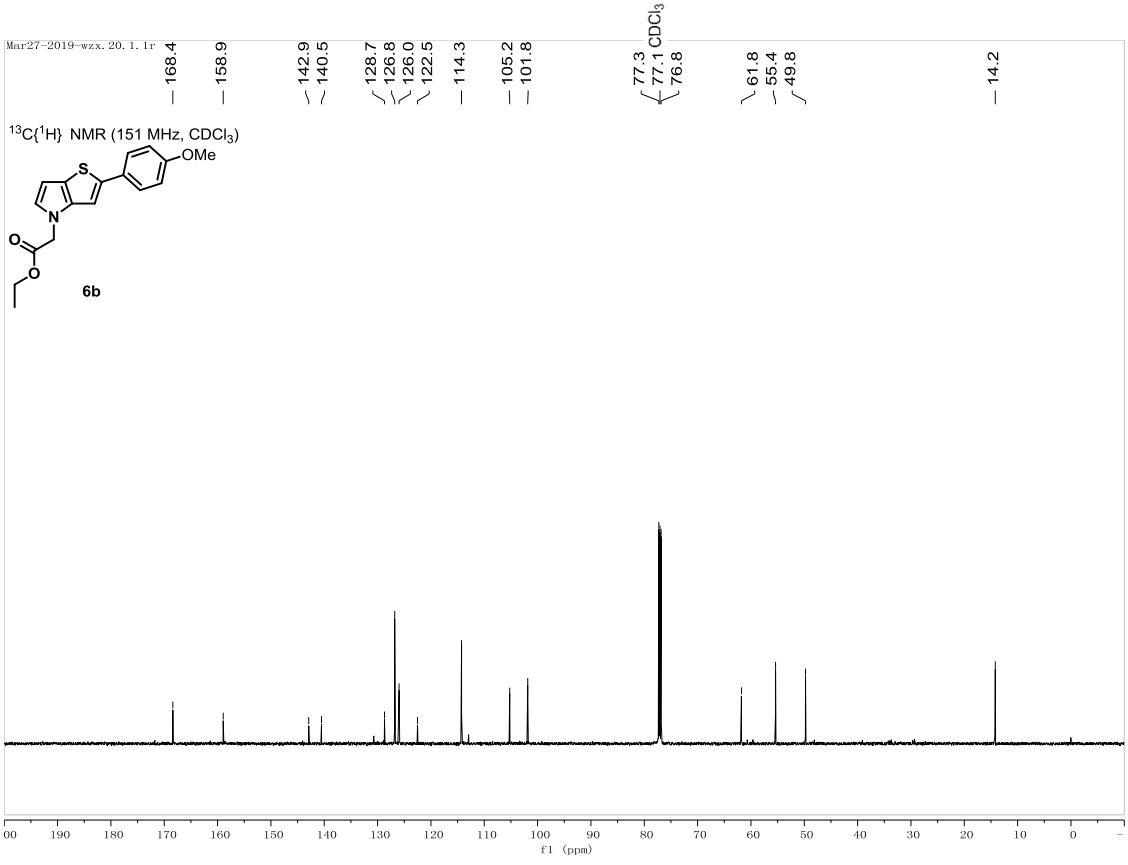

^{1}H NMR (400 MHz, $CDCl_3$)
4l
f1 (ppm)

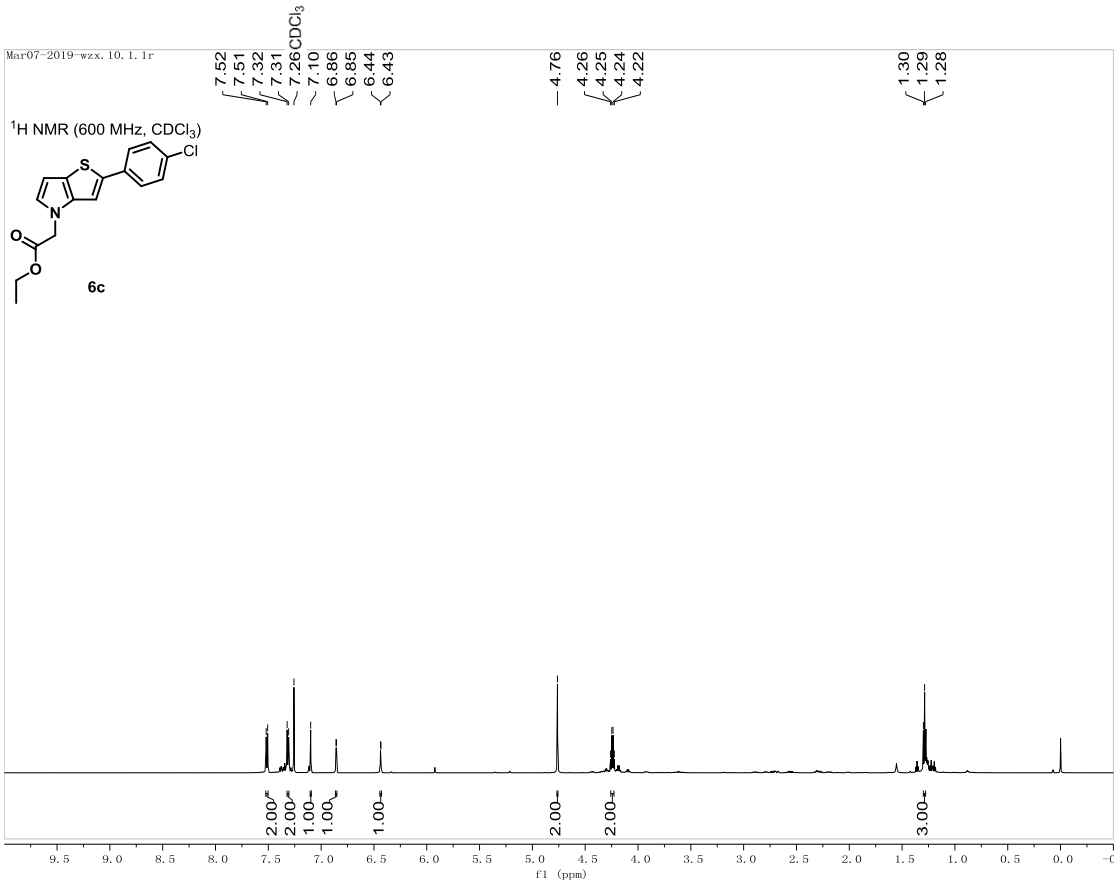

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)
4l
f1 (ppm)

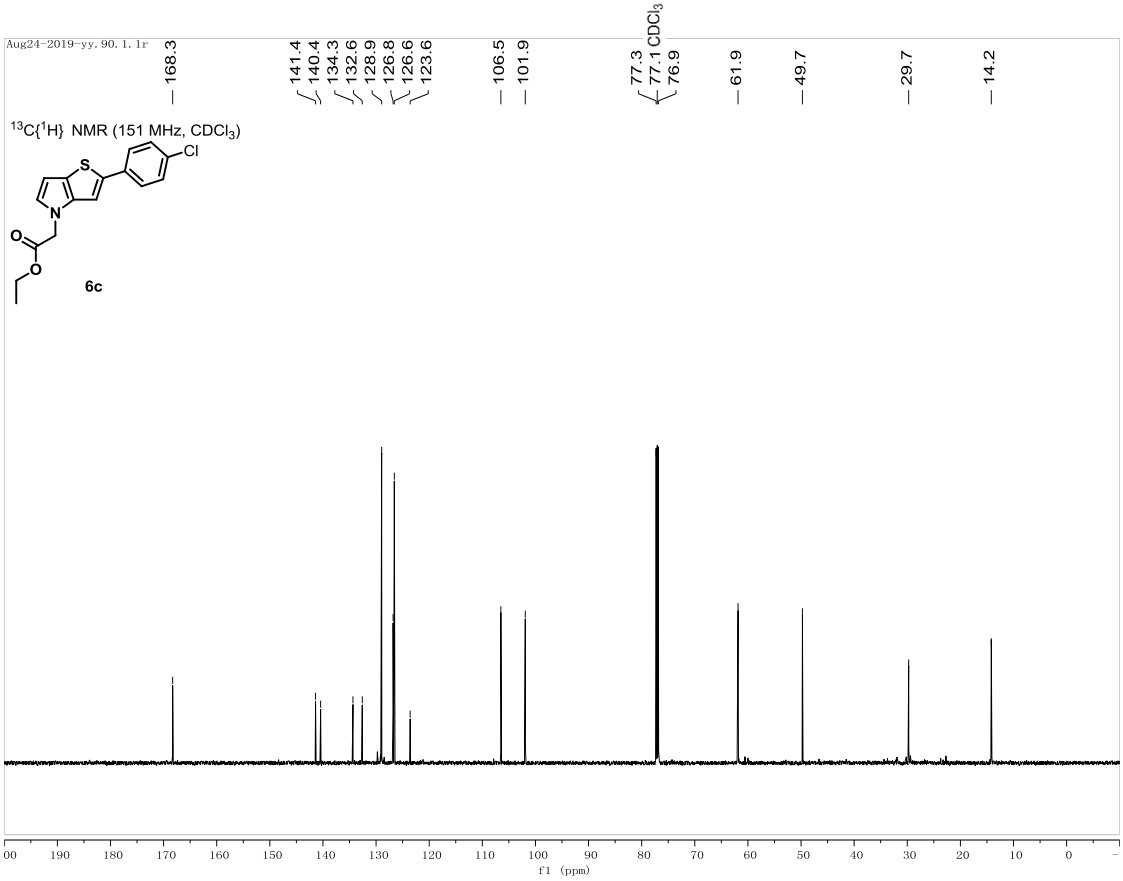

Feb23-2019-wzx. 10. 1. 1r
^{1}H NMR (600 MHz, CDCl$_3$)
6a
7.62
7.60
7.38
7.37
7.35
7.26 CDCl$_3$
7.25
7.23
7.14
6.86
6.85
6.45
6.45
4.77
4.27
4.26
4.24
4.23
1.31
1.29
1.28
2.00
2.00
1.00
1.00
1.00
2.00
2.00
3.00
f1 (ppm)

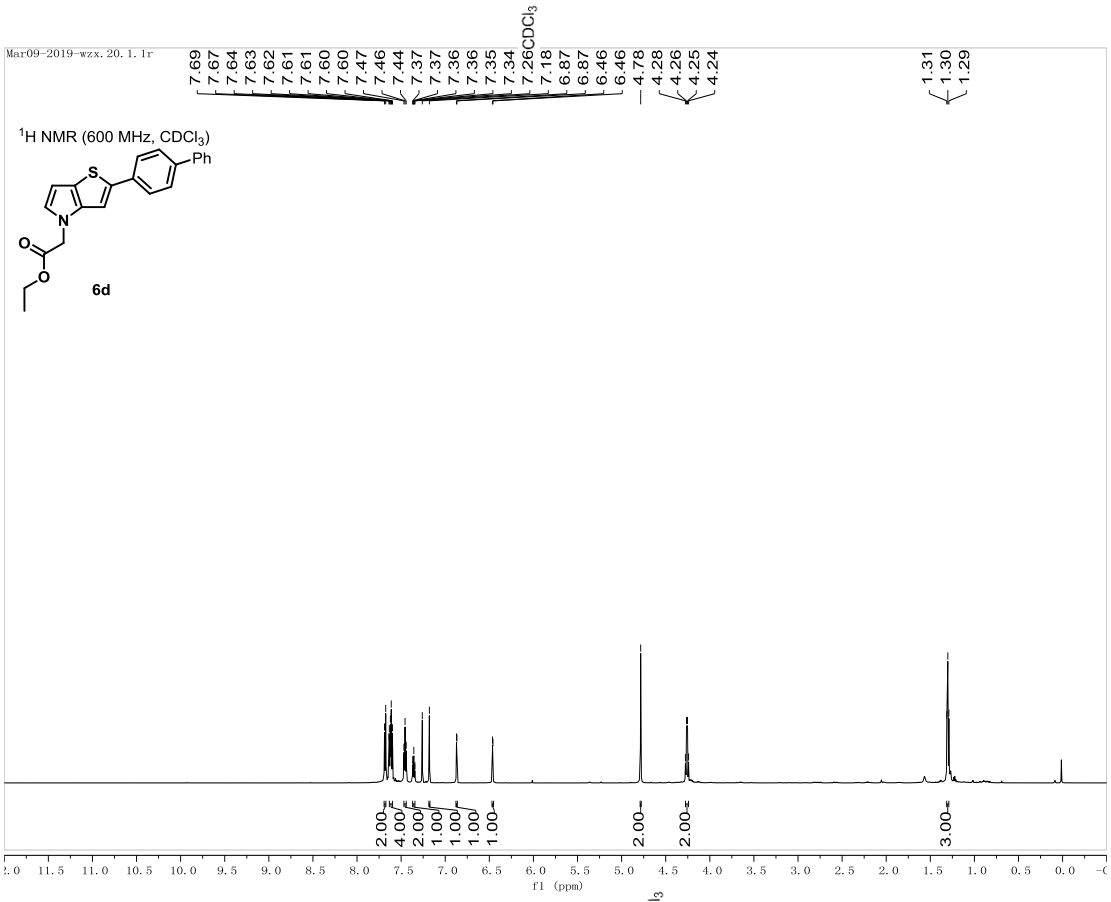

Mar27-2019-wzx. 10. 1. 1r
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$)
6a
168.3
142.9
140.5
135.8
128.8
127.0
126.5
125.5
123.3
106.1
101.9
77.3
77.1 CDCl$_3$
76.8
61.8
49.8
14.2
f1 (ppm)

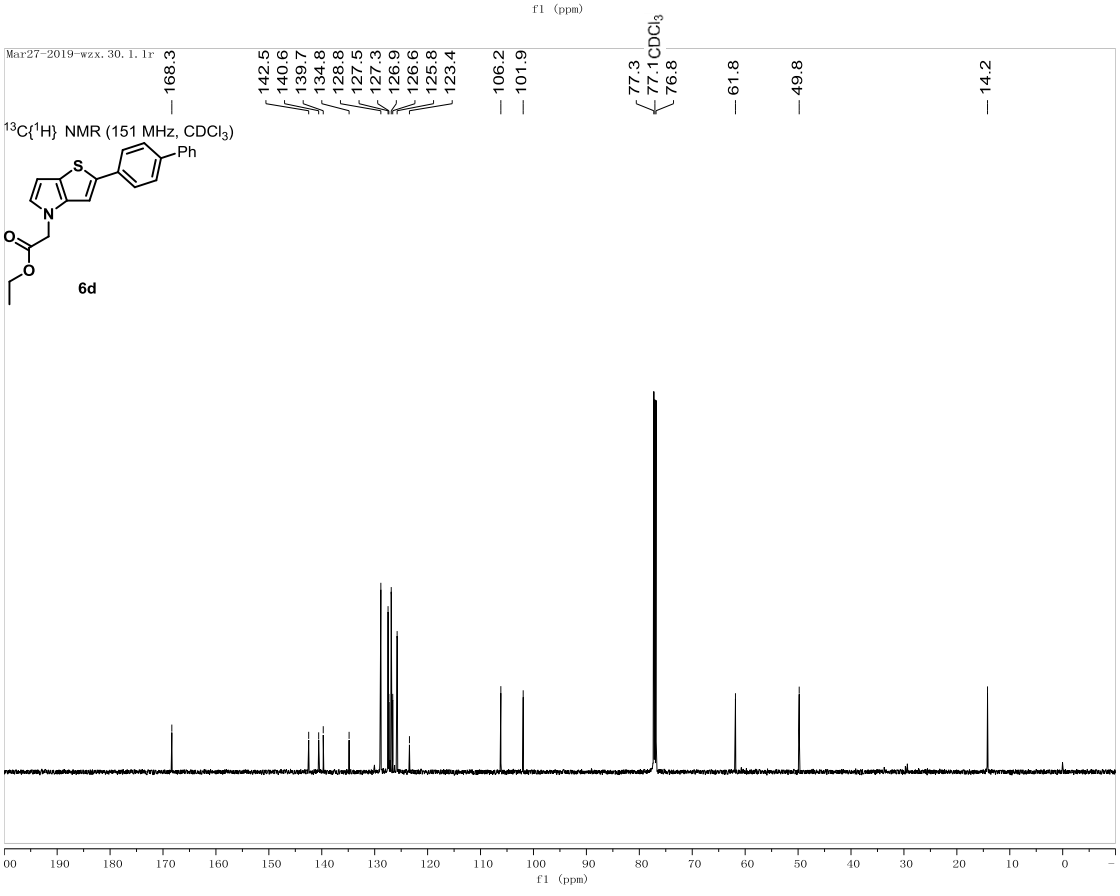

Mar02-2019-wzx. 20. 1. 1r
7.53
7.52
7.26CDCl3
7.01
6.91
6.90
6.83
6.82
6.43
6.42
4.76
4.26
4.25
4.24
4.22
3.83
1.30
1.29
1.28
1H NMR (600 MHz, CDCl3)
OMe
S
N
O
O
6b
2.00
1.00
2.00
1.00
1.00
2.00
2.00
3.00
3.00
f1 (ppm)

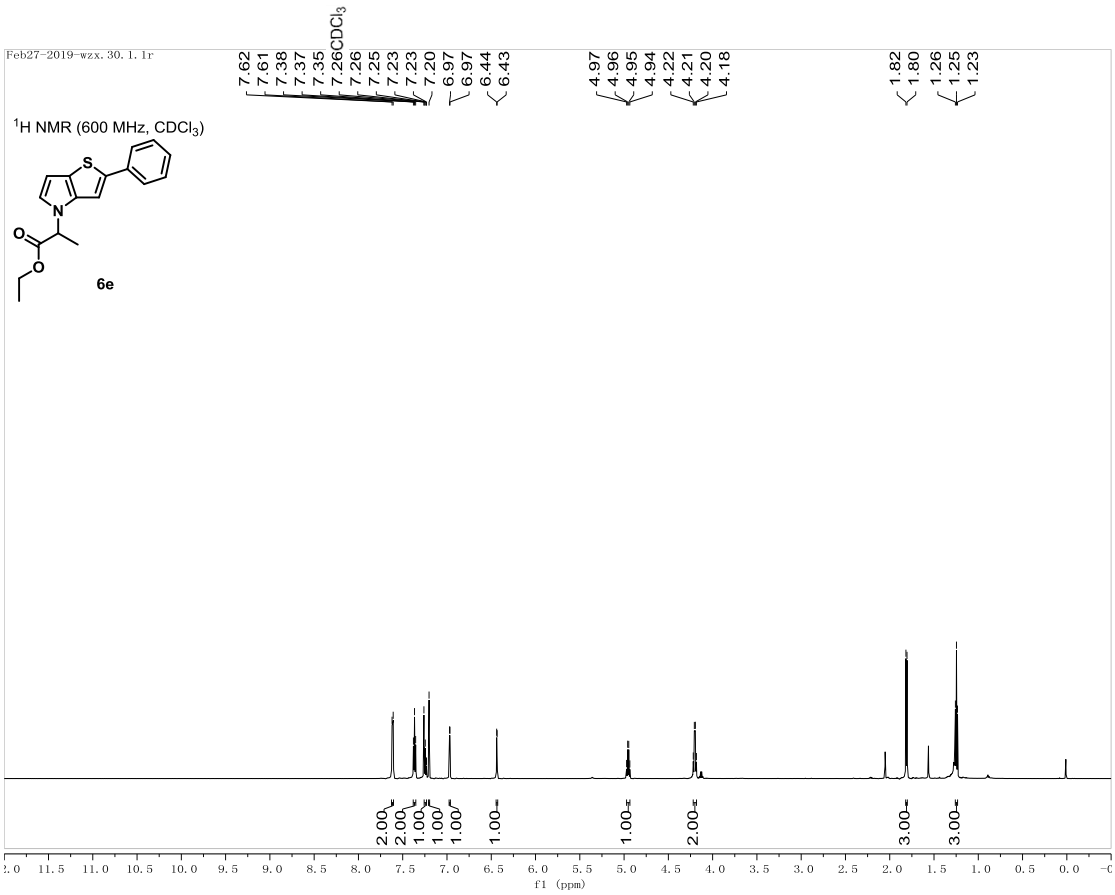

Mar27-2019-wzx. 20. 1. 1r
168.4
158.9
142.9
140.5
128.7
126.8
126.0
122.5
114.3
105.2
101.8
77.3
77.1 CDCl3
76.8
61.8
55.4
49.8
14.2
13C{1H} NMR (151 MHz, CDCl3)
OMe
S
N
O
O
6b
f1 (ppm)

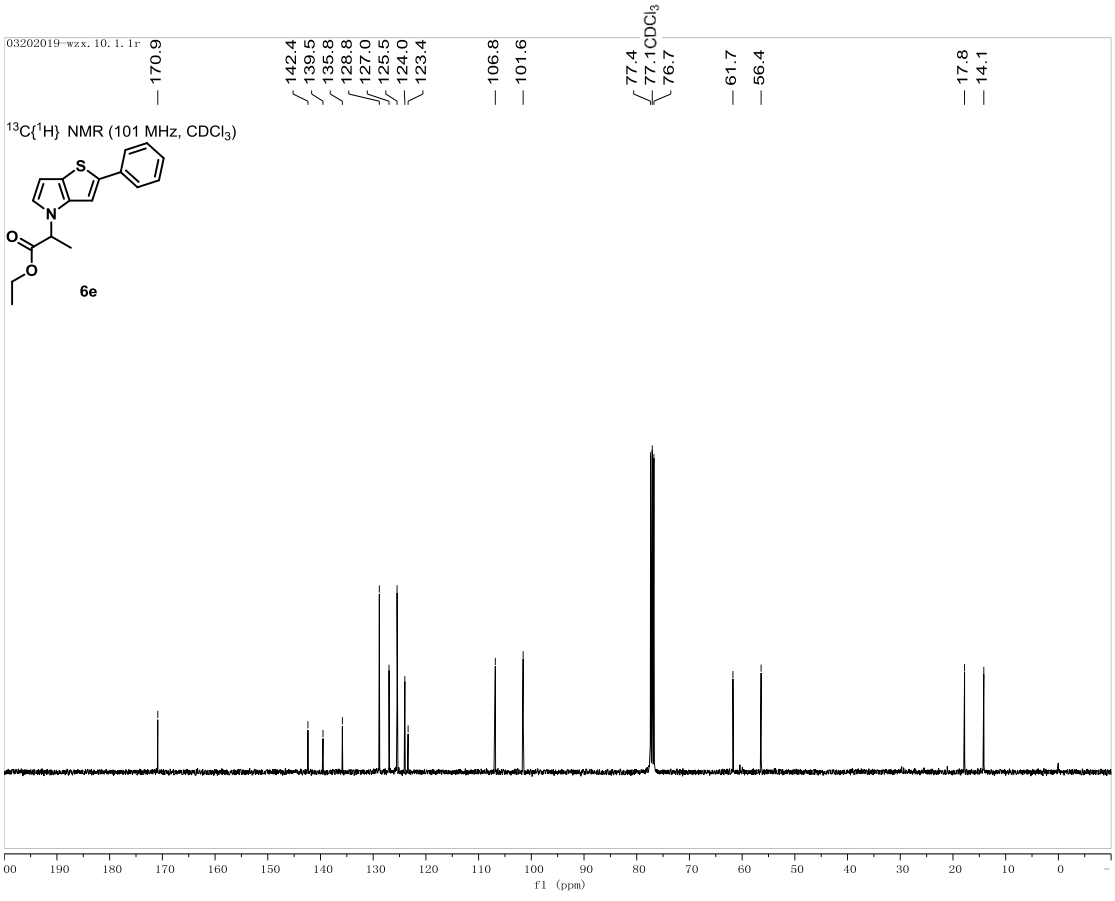

Mar07-2019-wzx. 10. 1. 1r
7.52
7.51
7.32
7.31
7.26 CDCl3
7.10
6.86
6.85
6.44
6.43
4.76
4.26
4.25
4.24
4.22
1.30
1.29
1.28
1H NMR (600 MHz, CDCl3)
Cl
S
N
O
O
6c
2.00
2.00
1.00
1.00
1.00
2.00
2.00
3.00
f1 (ppm)

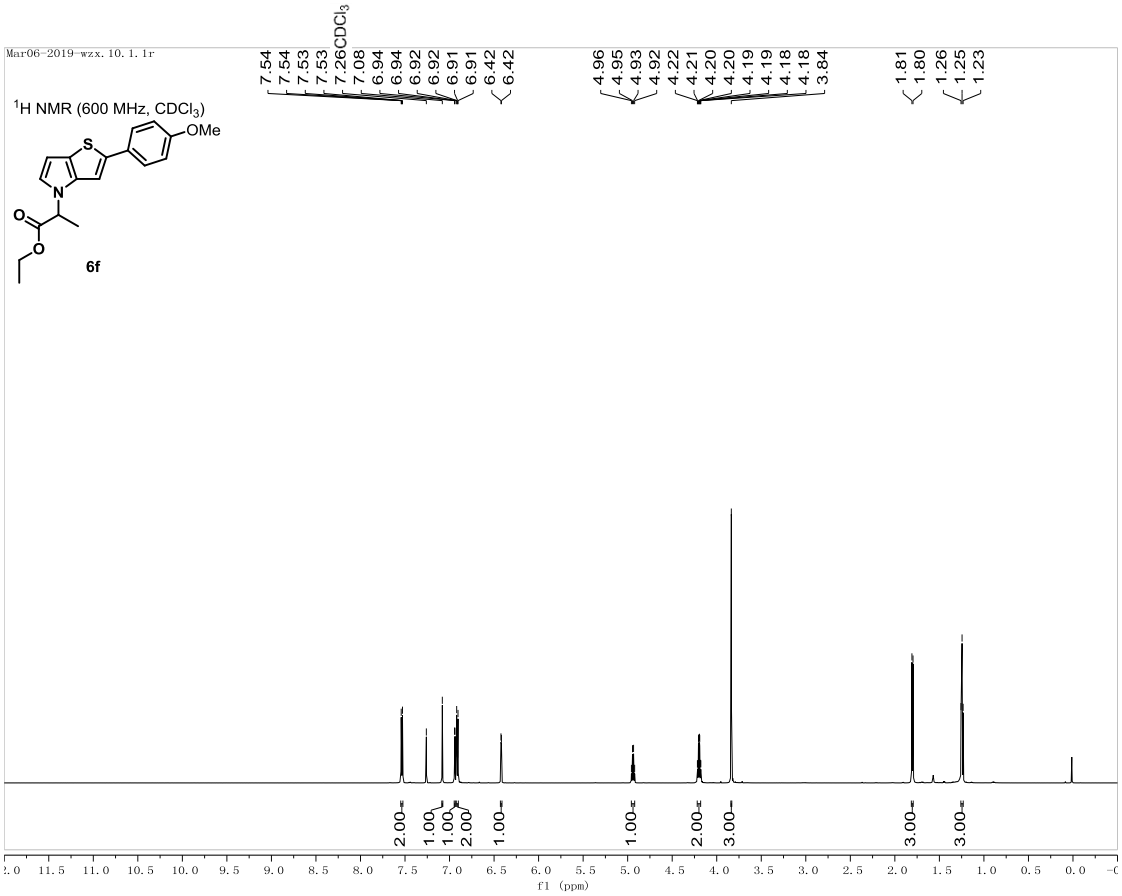

Aug24-2019-yy. 90. 1. 1r
168.3
141.4
140.4
134.3
132.6
128.9
126.8
126.6
123.6
106.5
101.9
77.3
77.1 CDCl3
76.9
61.9
49.7
29.7
14.2
13C{1H} NMR (151 MHz, CDCl3)
Cl
S
N
O
O
6c
f1 (ppm)

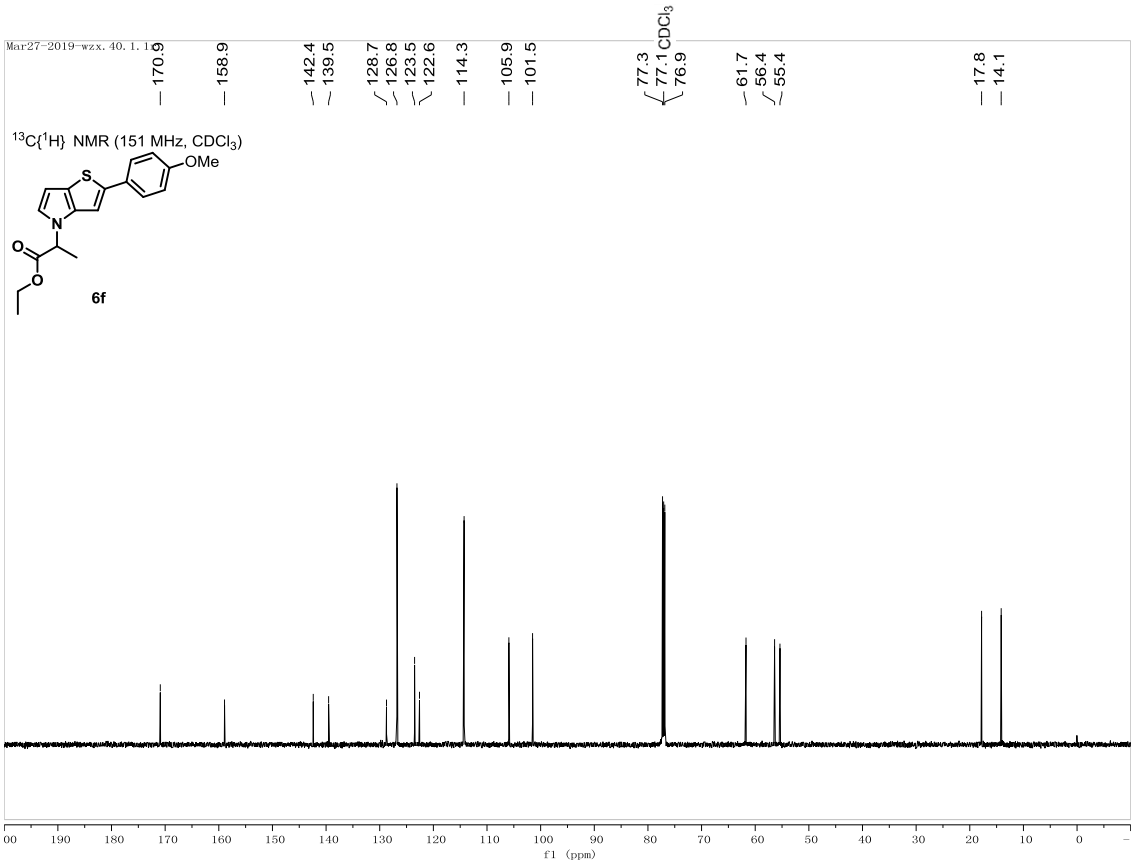

Mar09-2019-wzx.20.1.1r
7.69
7.67
7.64
7.63
7.62
7.61
7.61
7.60
7.60
7.47
7.46
7.44
7.37
7.37
7.36
7.36
7.35
7.34
7.26CDCl3
7.18
6.87
6.87
6.46
6.46
4.78
4.28
4.26
4.25
4.24
1.31
1.30
1.29
1H NMR (600 MHz, CDCl3)
Ph
S
N
O
O
6d
2.00
4.00
2.00
1.00
1.00
1.00
2.00
2.00
3.00
f1 (ppm)

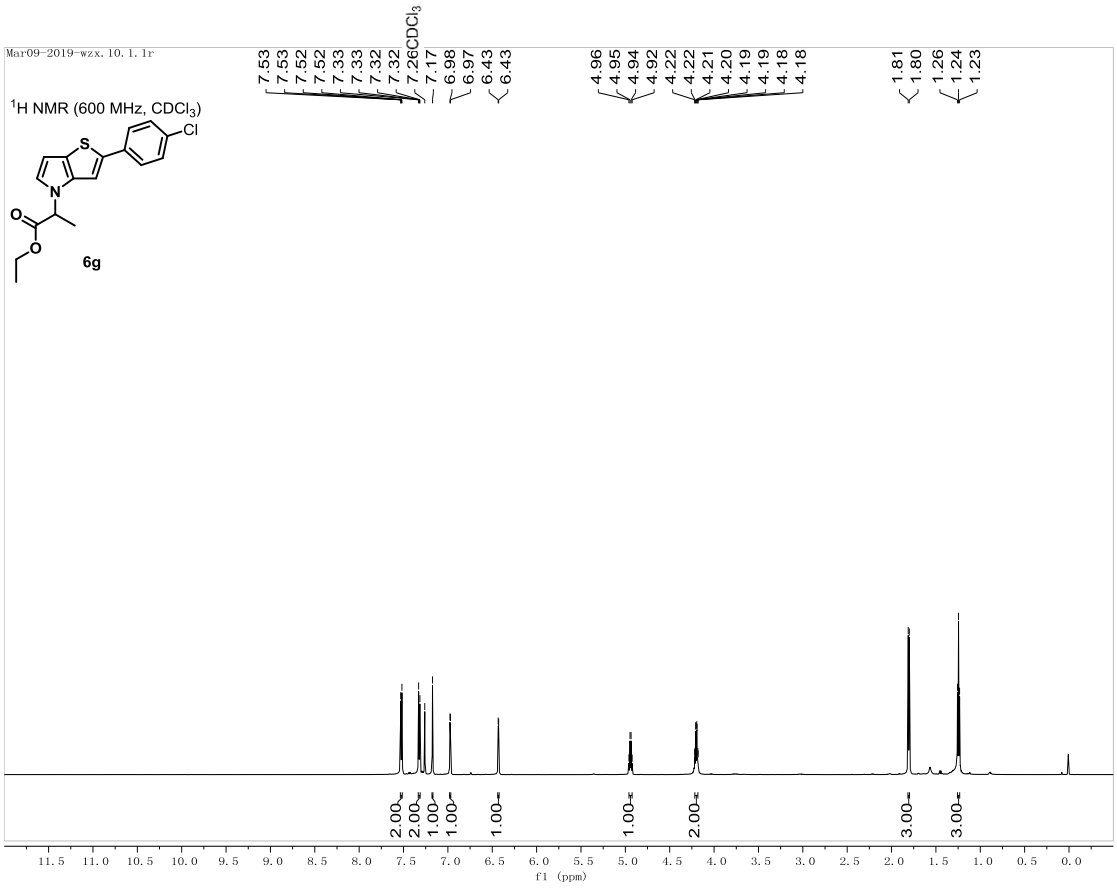

Mar27-2019-wzx.30.1.1r
168.3
142.5
140.6
139.7
134.8
128.8
127.5
127.3
126.9
126.6
125.8
123.4
106.2
101.9
77.3
77.1CDCl3
76.8
61.8
49.8
14.2
13C{1H} NMR (151 MHz, CDCl3)
Ph
S
N
O
O
6d
f1 (ppm)

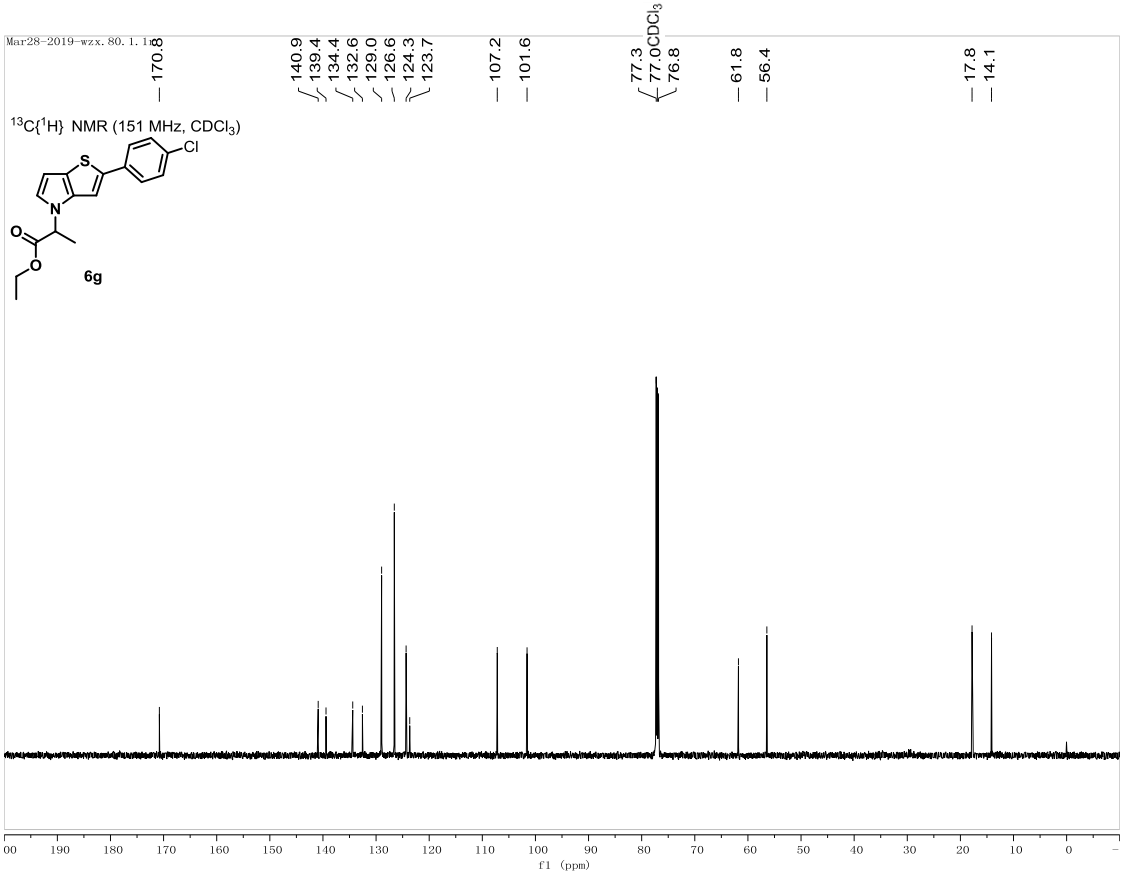

Feb27-2019-wzx. 30. 1. 1r
7.62
7.61
7.38
7.37
7.35
7.26CDCl3
7.26
7.25
7.23
7.23
7.20
6.97
6.97
6.44
6.43
4.97
4.96
4.95
4.94
4.22
4.21
4.20
4.18
1.82
1.80
1.26
1.25
1.23
1H NMR (600 MHz, CDCl3)
6e
2.00
2.00
1.00
1.00
1.00
1.00
1.00
2.00
3.00
3.00
f1 (ppm)

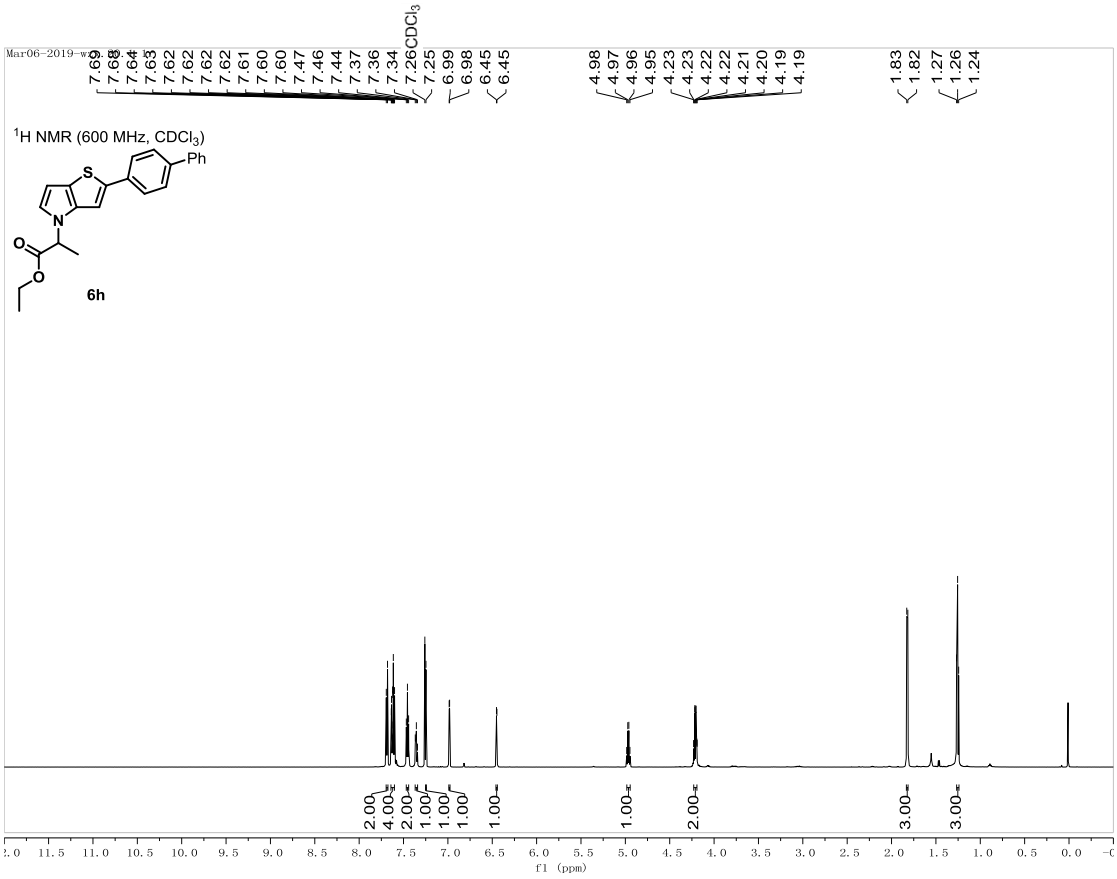

03202019-wzx. 10. 1. 1r
170.9
142.4
139.5
135.8
128.8
127.0
125.5
124.0
123.4
106.8
101.6
77.4
77.1CDCl3
76.7
61.7
56.4
17.8
14.1
13C{1H} NMR (101 MHz, CDCl3)
6e
f1 (ppm)

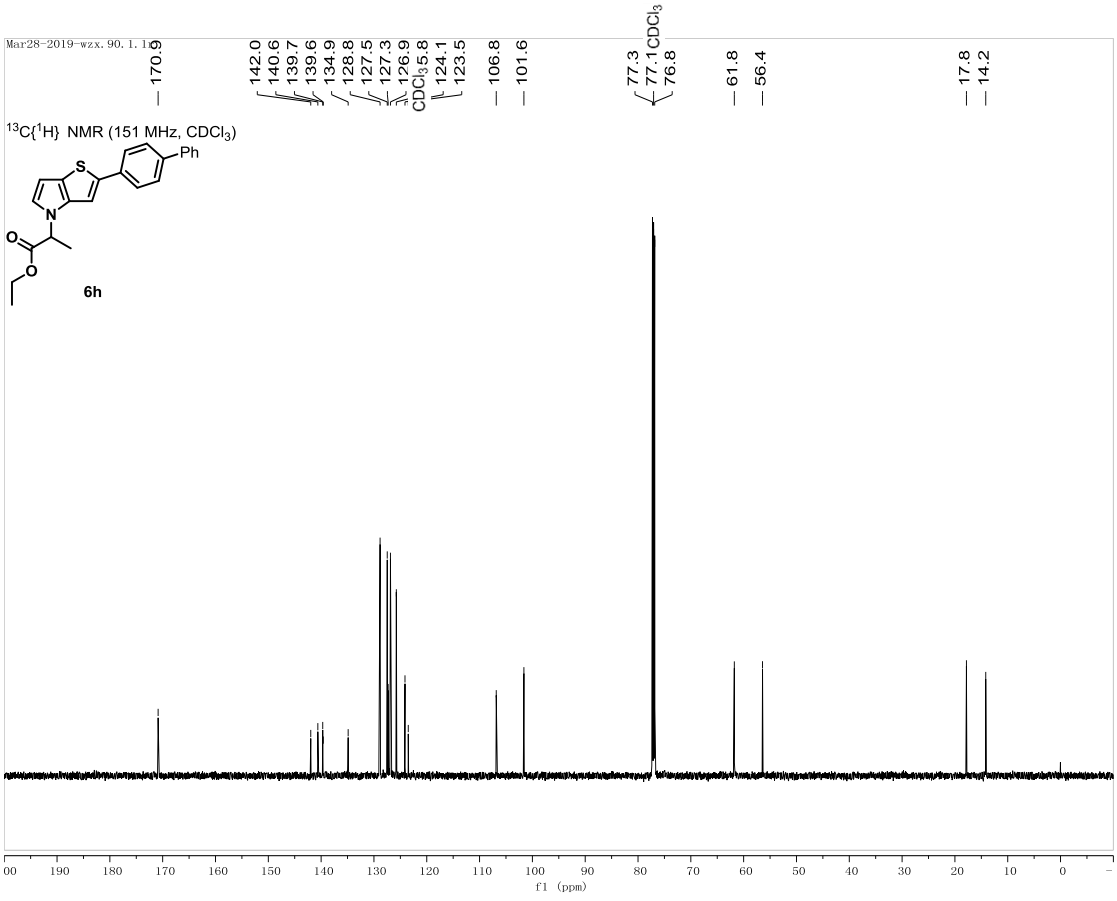

Mar06-2019-wzx. 10. 1. 1r
^{1}H NMR (600 MHz, CDCl$_3$)
OMe
S
N
O
O
6f
7.54
7.54
7.53
7.53
7.26CDCl$_3$
7.08
6.94
6.94
6.92
6.92
6.91
6.91
6.42
6.42
4.96
4.95
4.93
4.92
4.22
4.21
4.20
4.20
4.19
4.19
4.18
4.18
3.84
1.81
1.80
1.26
1.25
1.23
2.00
1.00
1.00
2.00
1.00
1.00
2.00
3.00
3.00
3.00
f1 (ppm)

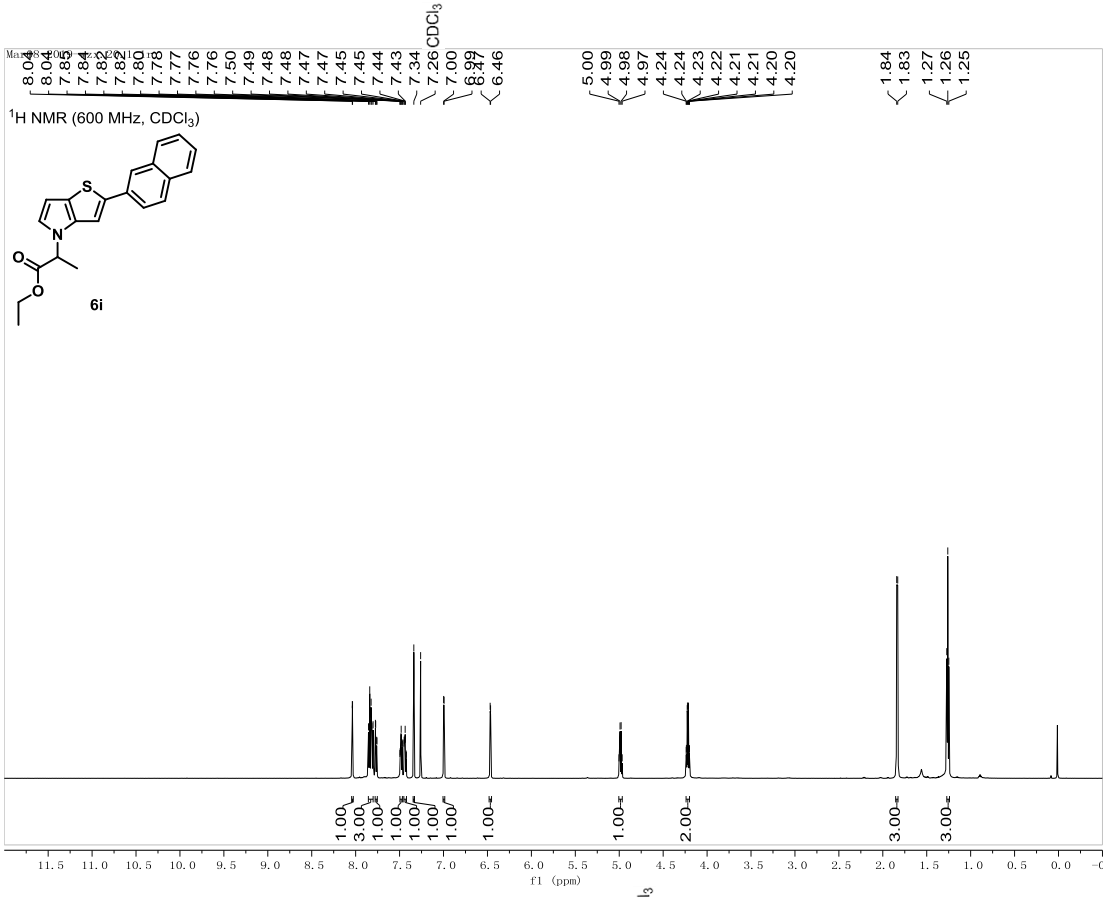

Mar27-2019-wzx. 40. 1. 1r
^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$)
OMe
S
N
O
O
6f
170.9
158.9
142.4
139.5
128.7
126.8
123.5
122.6
114.3
105.9
101.5
77.3
77.1 CDCl$_3$
76.9
61.7
56.4
55.4
17.8
14.1
f1 (ppm)


Mar09-2019-wzx. 10. 1. 1r
^{1}H NMR (600 MHz, $CDCl_3$)
6g
7.53 7.53 7.52 7.52 7.33 7.33 7.32 7.32 7.26 $CDCl_3$ 7.17 6.98 6.97 6.43 6.43
4.96 4.95 4.94 4.92 4.22 4.22 4.21 4.20 4.19 4.19 4.18 4.18
1.81 1.80 1.26 1.24 1.23
2.00 2.00 1.00 1.00 1.00 1.00 2.00 3.00 3.00
f1 (ppm)


Mar28-2019-wzx. 80. 1. 1r
$^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$)
6g
170.8
140.9 139.4 134.4 132.6 129.0 126.6 124.3 123.7
107.2 101.6
77.3 77.0 $CDCl_3$ 76.8
61.8 56.4
17.8 14.1
f1 (ppm)


Mar06-2019-wzx.90.1.1
7.69 7.68 7.64 7.63 7.62 7.62 7.62 7.61 7.60 7.60 7.47 7.46 7.44 7.37 7.36 7.34 7.26 CDCl3 7.25 6.99 6.98 6.45 6.45
4.98 4.97 4.96 4.95 4.23 4.23 4.22 4.22 4.21 4.20 4.19 4.19
1.83 1.82 1.27 1.26 1.24
1H NMR (600 MHz, CDCl3)
Ph
S
N
O
O
6h
2.00 4.00 2.00 1.00 1.00 1.00 1.00 1.00 2.00 3.00 3.00
f1 (ppm)


Mar28-2019-wzx.90.1.1
170.9
142.0 140.6 139.7 139.6 134.9 128.8 127.5 127.3 126.9 CDCl3 5.8 124.1 123.5
106.8 101.6
77.3 77.1 CDCl3 76.8
61.8 56.4
17.8 14.2
13C{1H} NMR (151 MHz, CDCl3)
Ph
S
N
O
O
6h
f1 (ppm)


8.04
8.04
7.85
7.84
7.82
7.82
7.80
7.78
7.77
7.76
7.76
7.50
7.49
7.48
7.48
7.47
7.47
7.45
7.45
7.44
7.43
7.34
7.26
CDCl3
7.00
6.99
6.47
6.46
5.00
4.99
4.98
4.97
4.24
4.24
4.23
4.22
4.21
4.21
4.20
4.20
1.84
1.83
1.27
1.26
1.25
1H NMR (600 MHz, CDCl3)
6i
1.00
3.00
1.00
1.00
1.00
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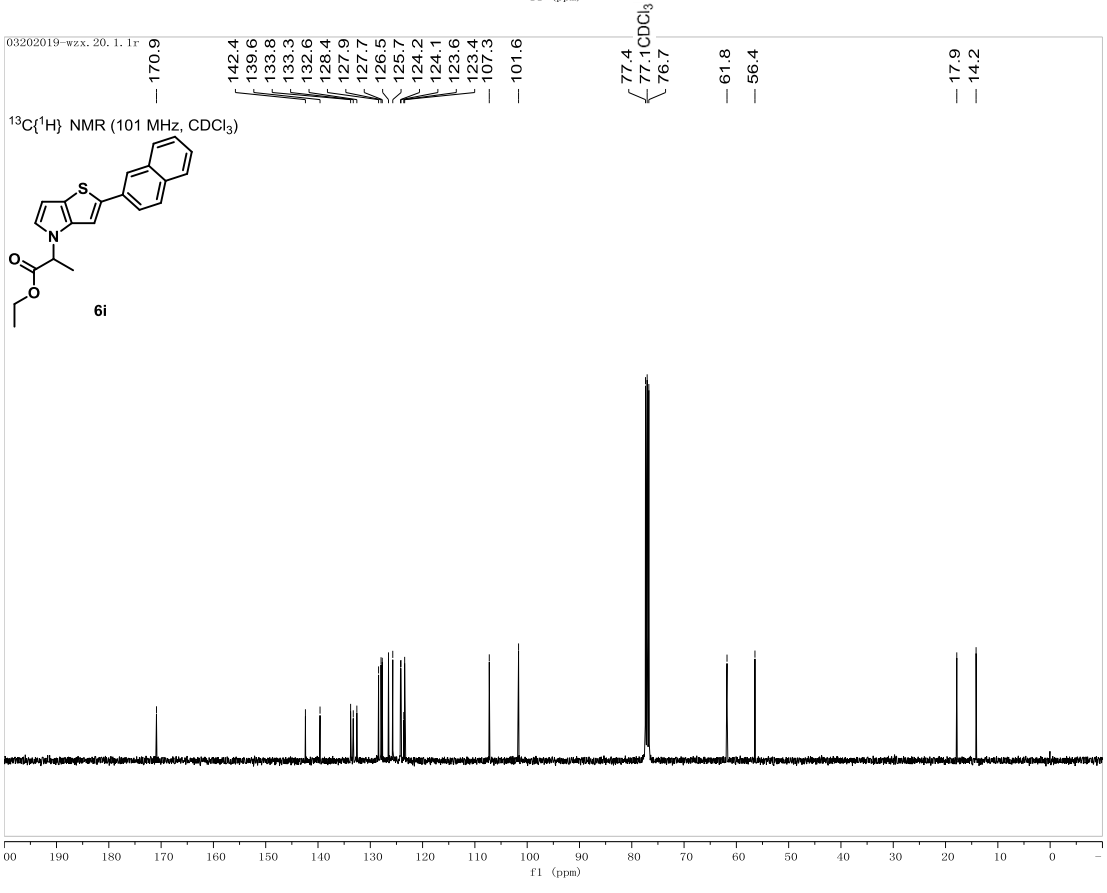
1.00
1.00
1.00
2.00
3.00
3.00
f1 (ppm)


03202019-wzx.20.1.1r
170.9
142.4
139.6
133.8
133.3
132.6
128.4
127.9
127.7
126.5
125.7
124.2
124.1
123.6
123.4
107.3
101.6
77.4
77.1
CDCl3
76.7
61.8
56.4
17.9
14.2
13C{1H} NMR (101 MHz, CDCl3)
6i
f1 (ppm)

5. Single-Crystal X-ray diffraction.

Single-crystal XRD studies on compounds **2b** and **2h** were performed on a Supernova CCD diffractometer at 293(2) K. Determination of unit cell parameters and data collection were performed with Mo-Ka radiation at a wavelength of 0.71073 Å using the x-scan technique. The structures were solved by direct methods and refined by full matrix least-squares on F^2 using SHELXS-97 and SHELXL-97 programs.[1] The metal atoms in each compound were located from the E-maps, and other non-hydrogen atoms were located in successive difference Fourier syntheses and refined with anisotropic thermal parameters on F^2. The hydrogen atoms were added theoretically, riding on the concerned atoms and refined with fixed thermal factors. The SQUEEZE function in PLATON was utilized during the refinement of **2b** and **2h** owing to the disordered solvents.[2]

The structure was then refined again using the data generated. Crystal data and details of the data collection are given in **Table S1-S2**. CCDC 1946767 (**2b**) and 1946766 (**2h**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

(1) M. Sheldrick, G. SHELXS-97. Program for X-ray crystal structure determination, Gottingen University, Germany, **1997**.

(2) L. Spek, A. Single-crystal structure validation with the program PLATON. *J. Appl. Crystallogr.* **2003**, *36*, 7-13.

Single crystals (**2b** and **2h**) suitable for X-ray analysis were obtained by slow evaporation of CH_2Cl_2 solvent.

Table S1. Crystal data and structure refinement for 2b

Identification code	shs-20180927
Empirical formula	$C_{20}H_{17}NS$
Formula weight	303.41
Temperature/K	293(2) K
Crystal system	monoclinic
Space group	P 1 21/c 1
a/Å	13.4137(6) A

b/Å	5.9329(2) A
c/Å	20.1416(8) A
α/°	90
β/°	90.210(4)
γ/°	90
Volume/Å^3	1602.90(11)
Z	4
ρ_{calc}g/cm^3	1.257
μ/mm^{-1}	0.198
F(000)	640
Crystal size/mm^3	0.45 ×0.28×0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.58 to 29.21
Index ranges	-17<=h<=16, -8<=k<=6, -26<=l<=25
Reflections collected	8879 / 3702 [R(int) = 0.0224]
Independent reflections	unique 3702
Data/restraints/parameters	3702 / 0 / 200
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R1 = 0.0439, wR2 = 0.0992
Final R indexes [all data]	R1 = 0.0604, wR2 = 0.1081
Largest diff. peak/hole / e Å^{-3}	0.218 and -0.236

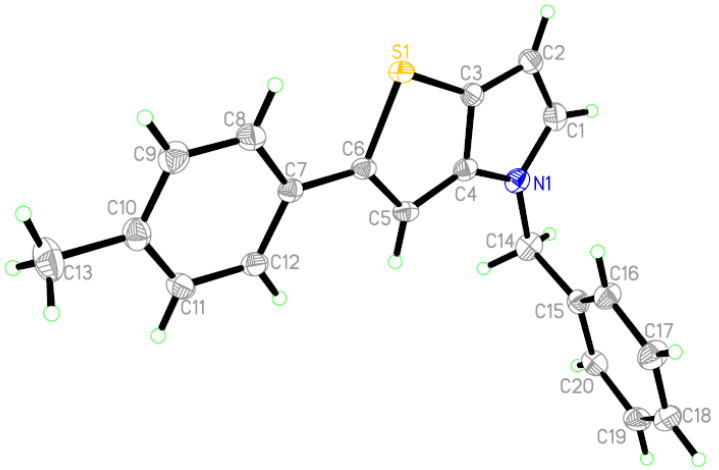


Figure S1. Additional X-ray crystallographic structures **2b** with 30% probability ellipsoid.

Table S2. Crystal data and structure refinement for 2h

Identification code	shs-2-20180919
Empirical formula	$C_{21}H_{19}NOS$
Formula weight	333.43
Temperature/K	293(2) K

Crystal system	monoclinic
Space group	C1c1
a/Å	28.9068(5) A
b/Å	5.75310(10) A
c/Å	10.5484(2) A
α/°	90
β/°	98.531(2)
γ/°	90
Volume/$Å^3$	1734.83(5)
Z	4
$\rho_{calc}g/cm^3$	1.277
μ/mm^{-1}	1.694
F(000)	704
Crystal size/mm^3	0.20 ×0.20 ×0.20
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.19 to 71.18
Index ranges	-34<=h<=35, -5<=k<=6, -12<=l<=9
Reflections collected	5226 / 2646 [R(int) = 0.0166]
Independent reflections	unique 2646
Data/restraints/parameters	2646 / 2 / 218
Goodness-of-fit on F^2	1.079
Final R indexes [I>=2σ (I)]	R1 = 0.0363, wR2 = 0.1052
Final R indexes [all data]	R1 = 0.0369, wR2 = 0.1060
Largest diff. peak/hole / e $Å^{-3}$	0.108 and -0.191

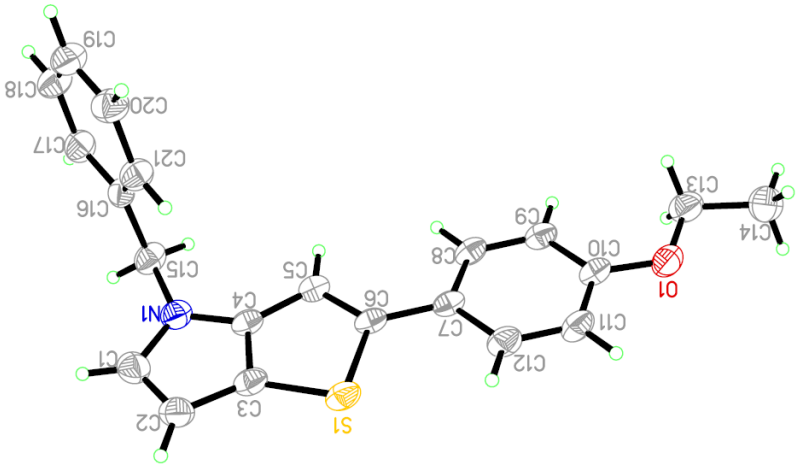


Figure S2. Additional X-ray crystallographic structures **2h** with 30% probability ellipsoid.