# SUPPORTING INFORMATION

## Synthesis of Sulfonamide-Based Ynamides and Ynamines in Water

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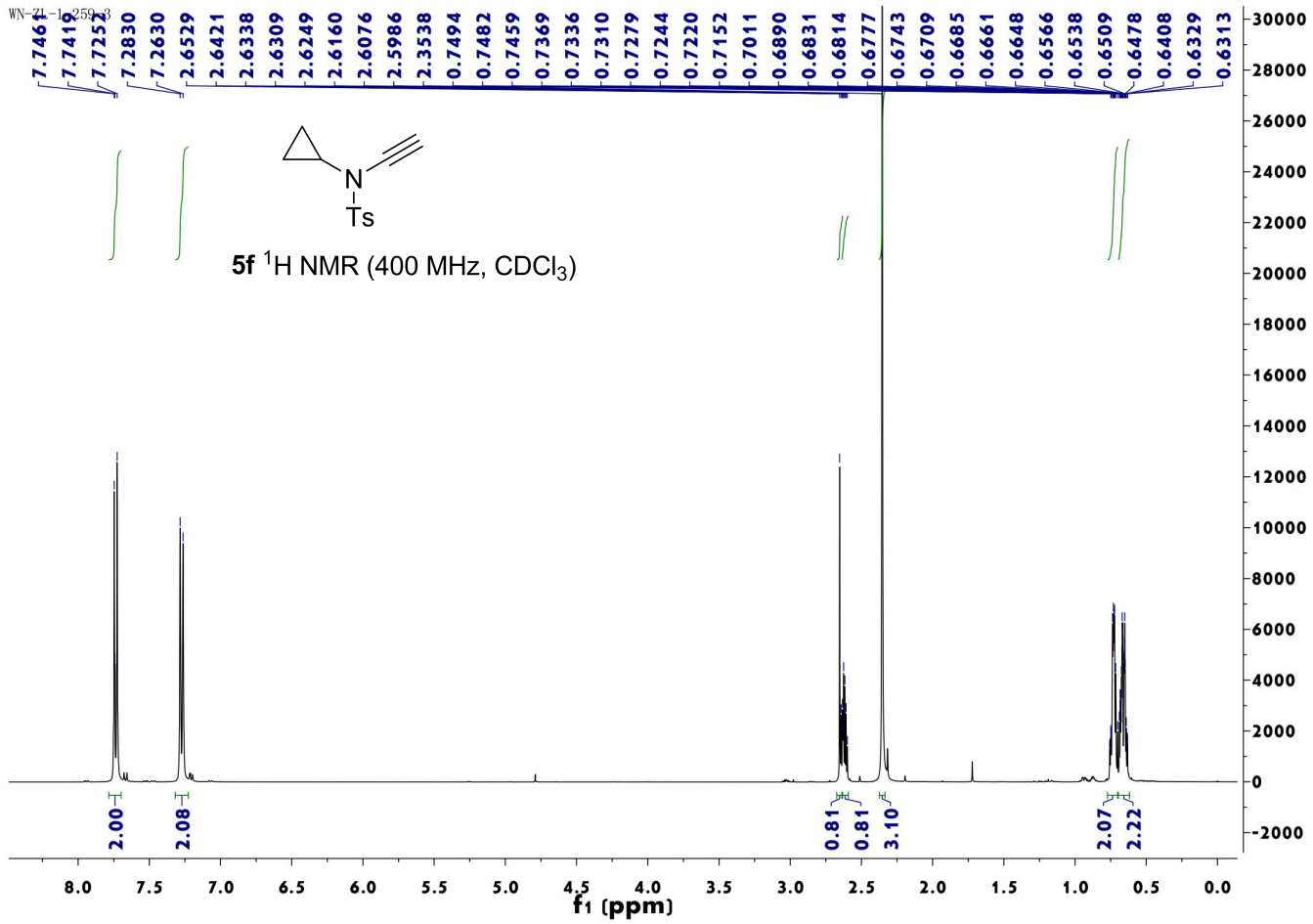
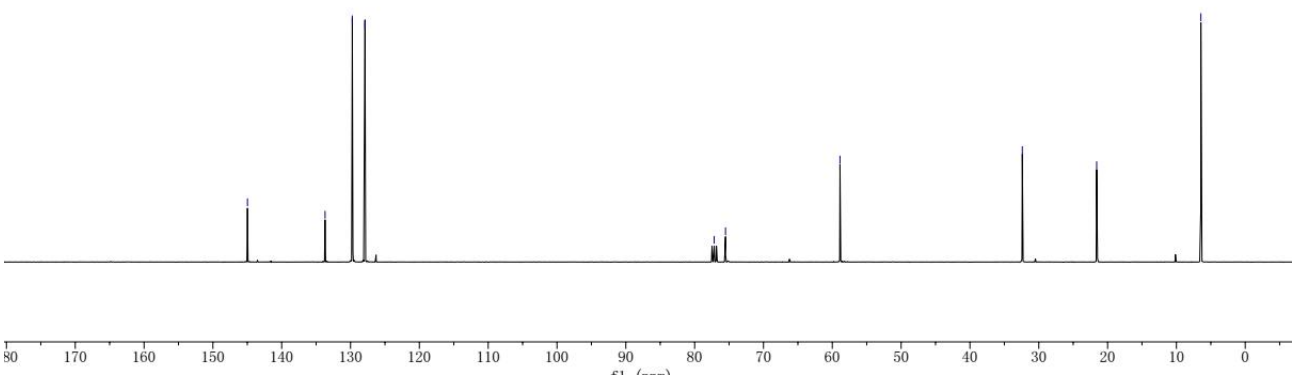
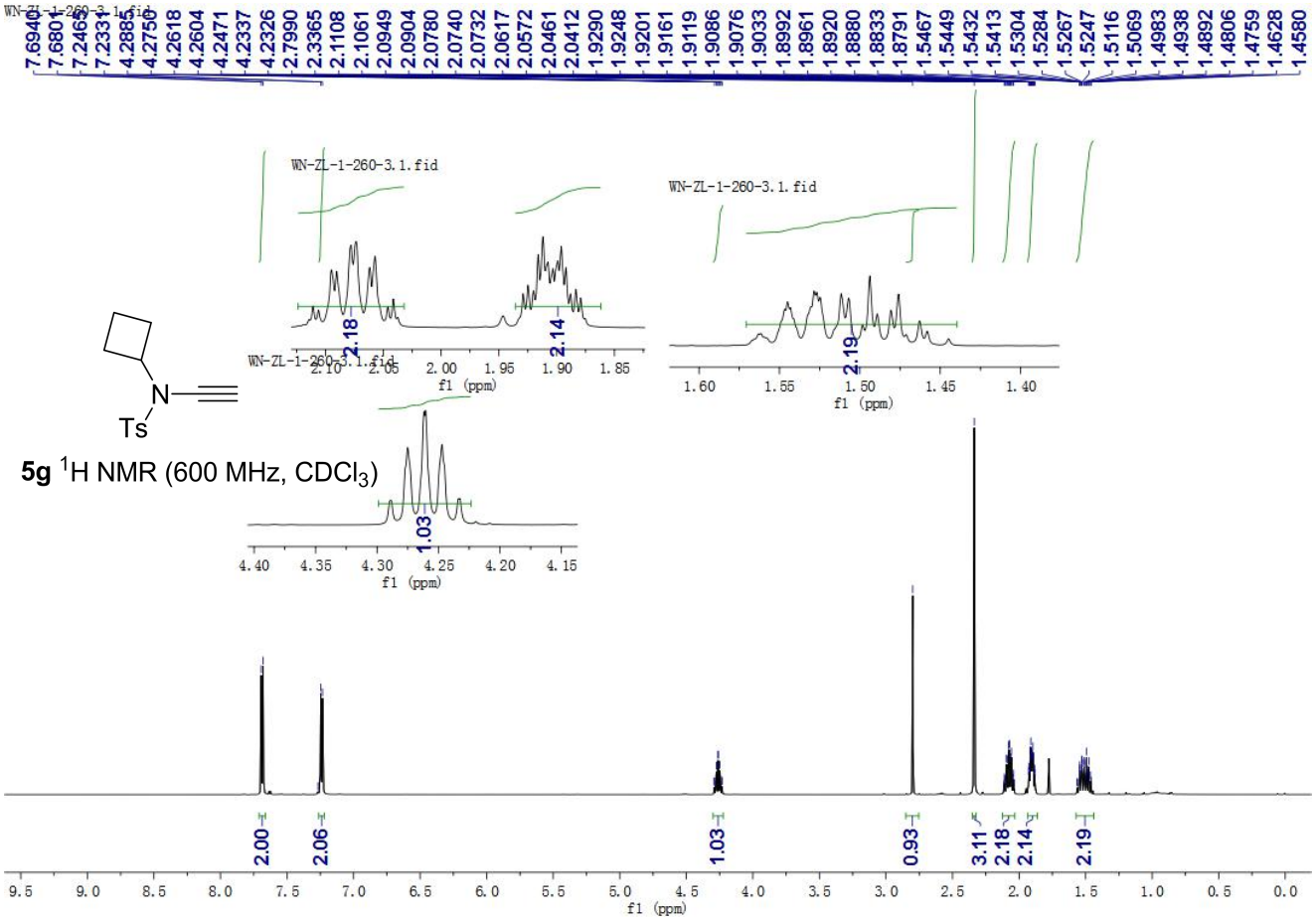
## 1. $^{1}H$ and $^{13}C$ NMR spectra



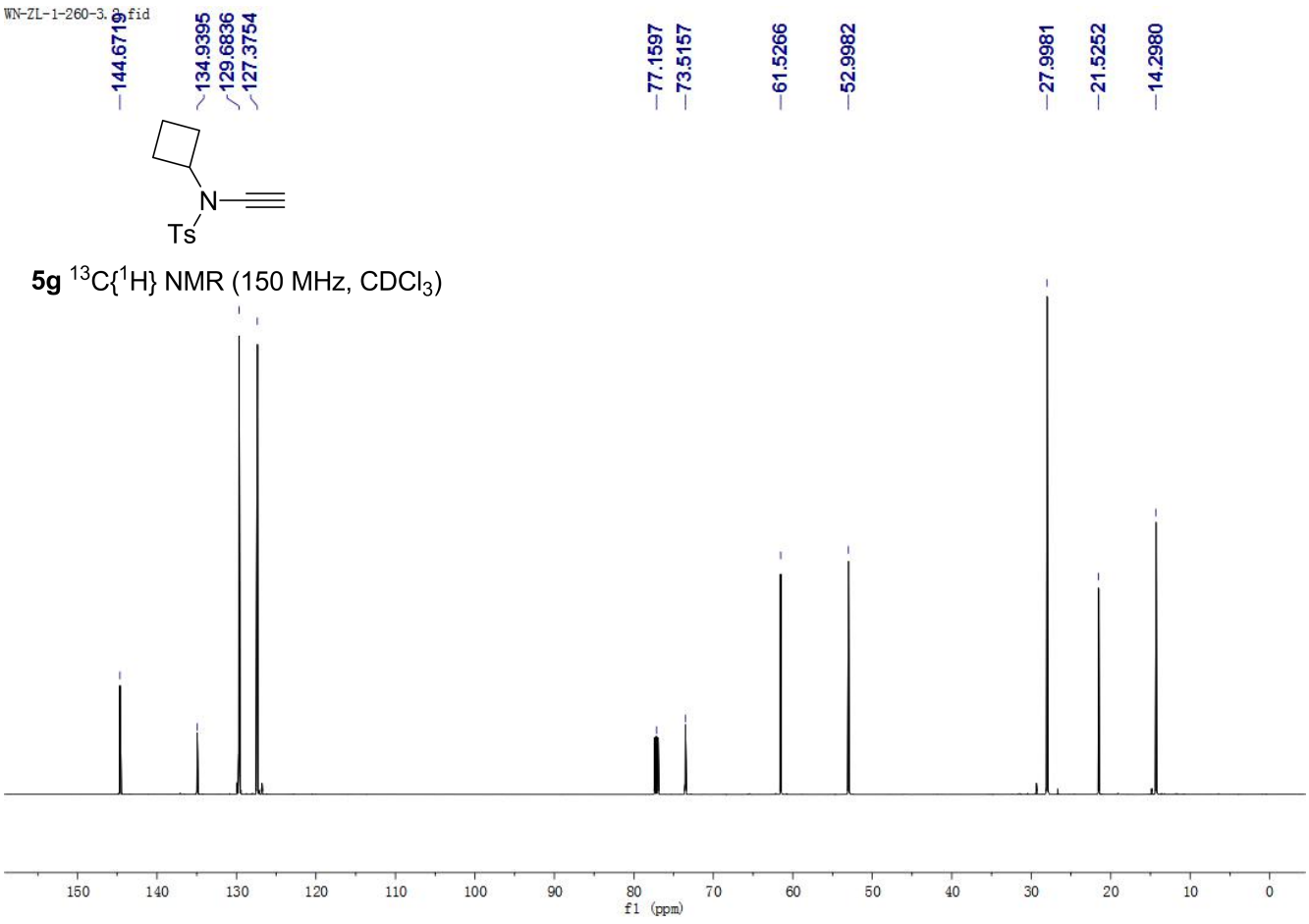

**5f** $^{1}H$ NMR (400 MHz, $CDCl_3$)


**5f** $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

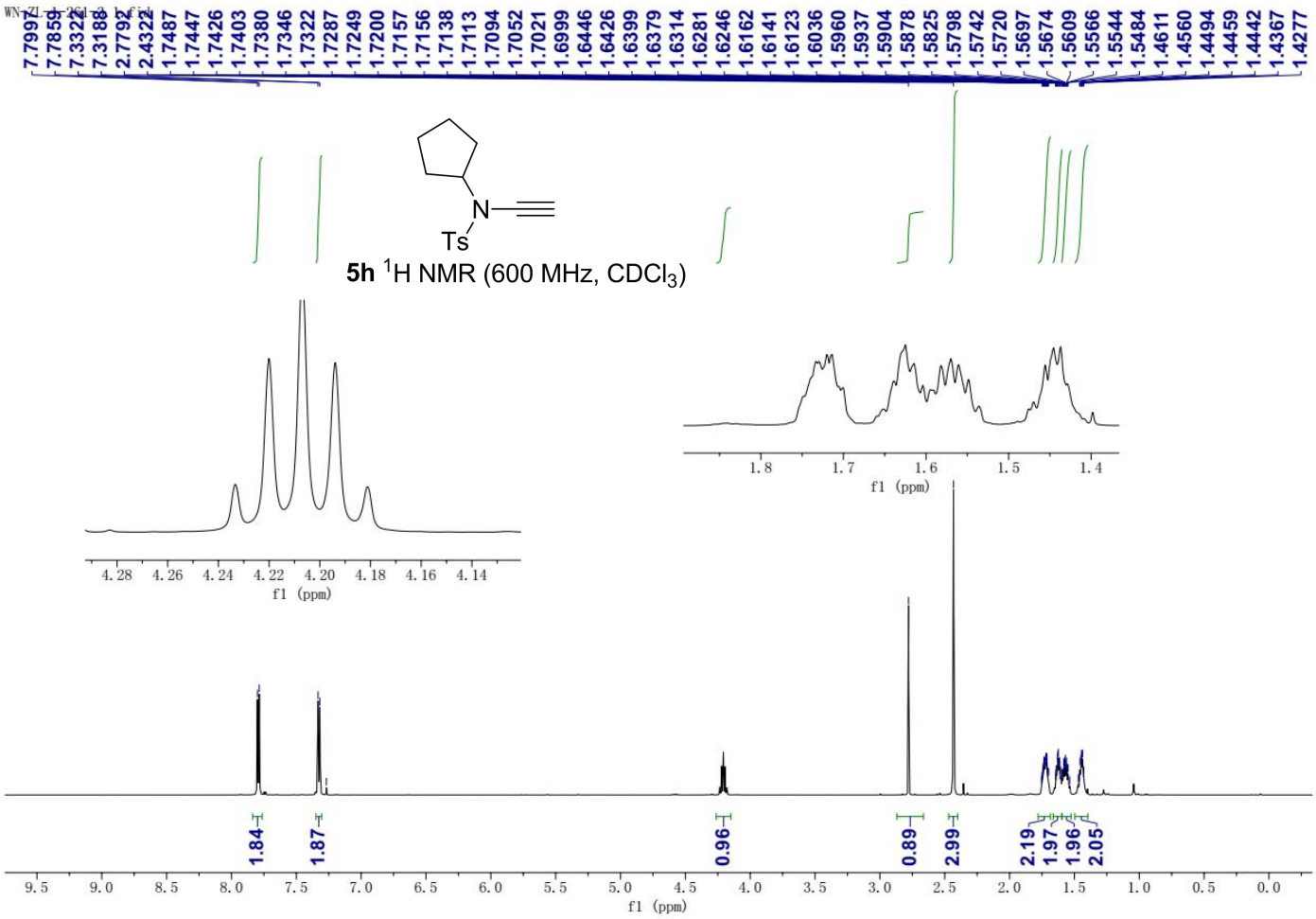





**5g** $^{1}$H NMR (600 MHz, $CDCl_3$)

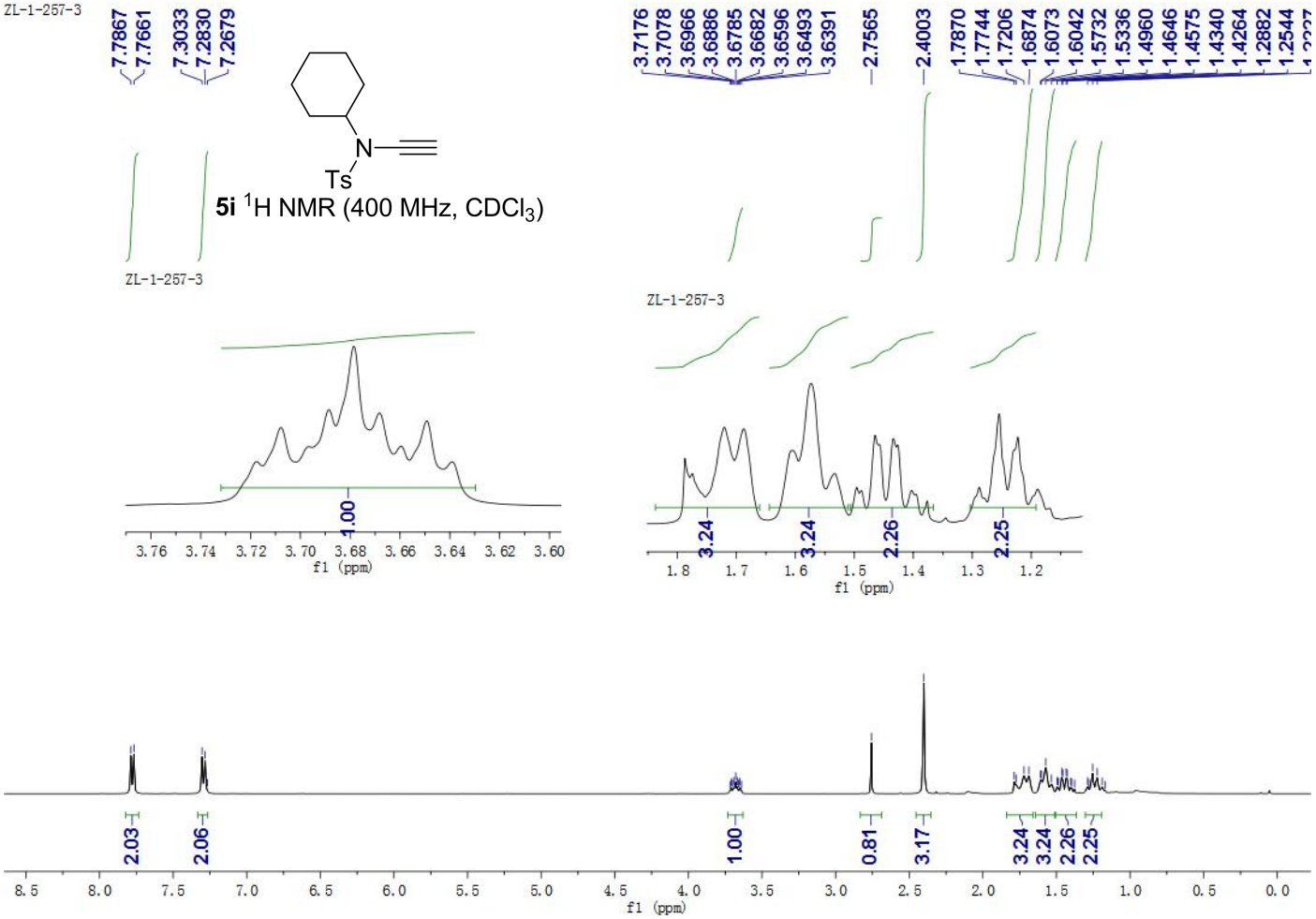



**5g** $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$)



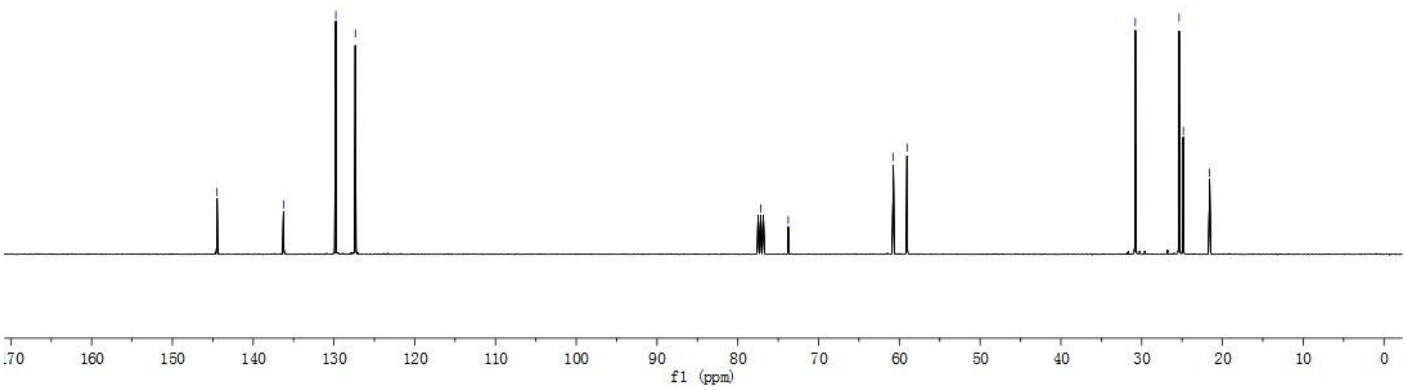

**5h** $^{1}$H NMR (600 MHz, $CDCl_3$)

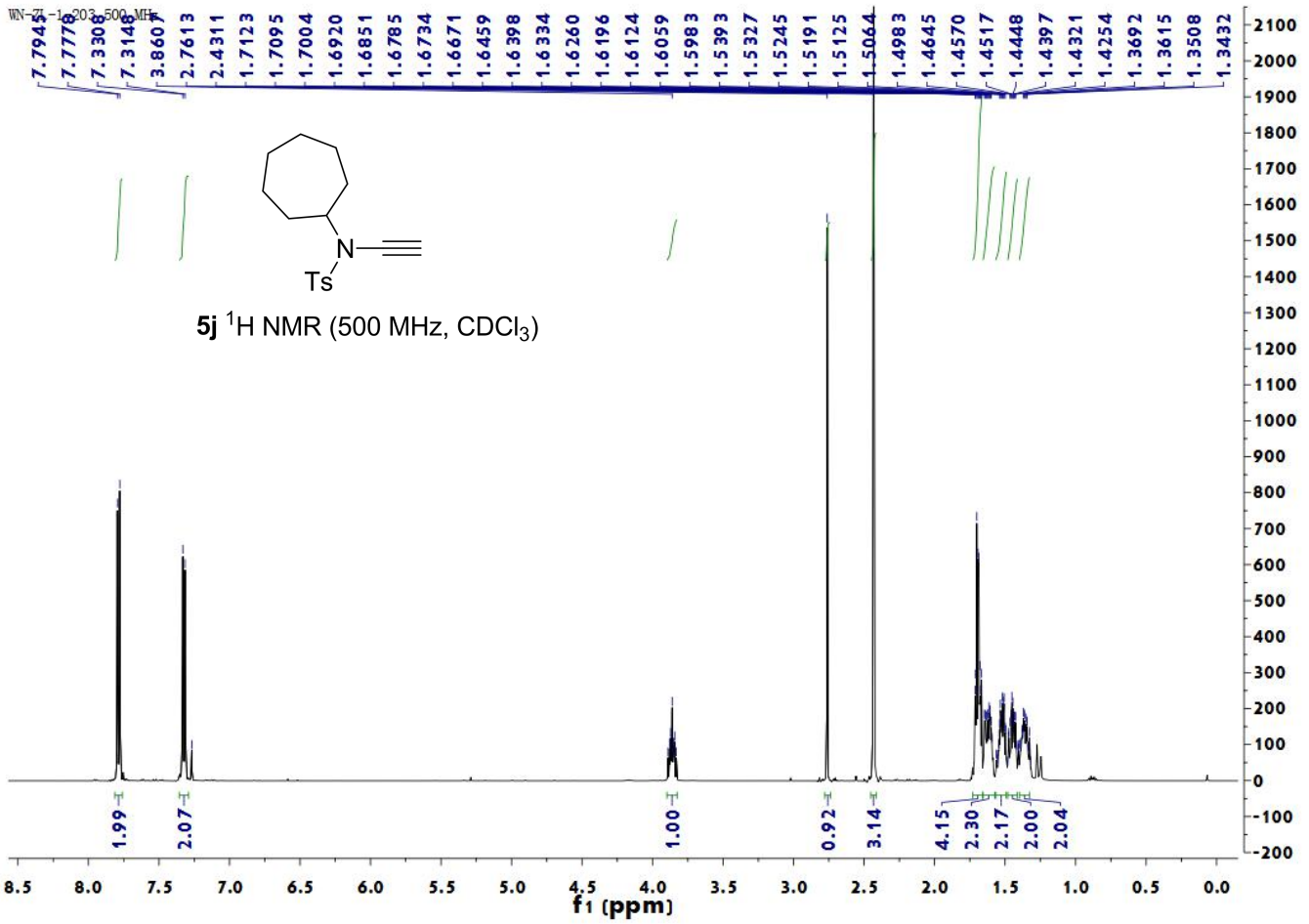

**5h** $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$)



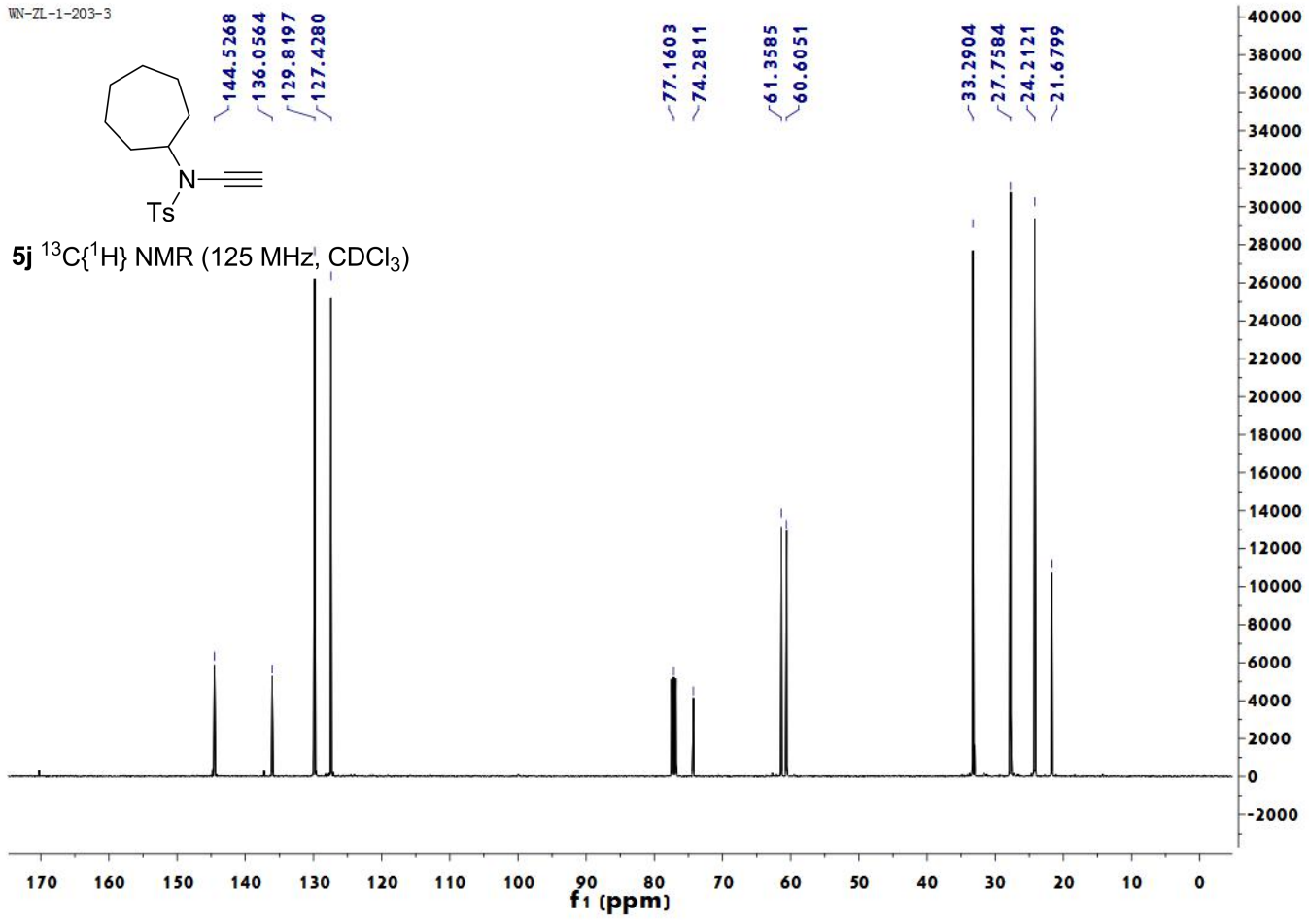

**5i** $^{1}$H NMR (400 MHz, $CDCl_3$)


**5i** $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

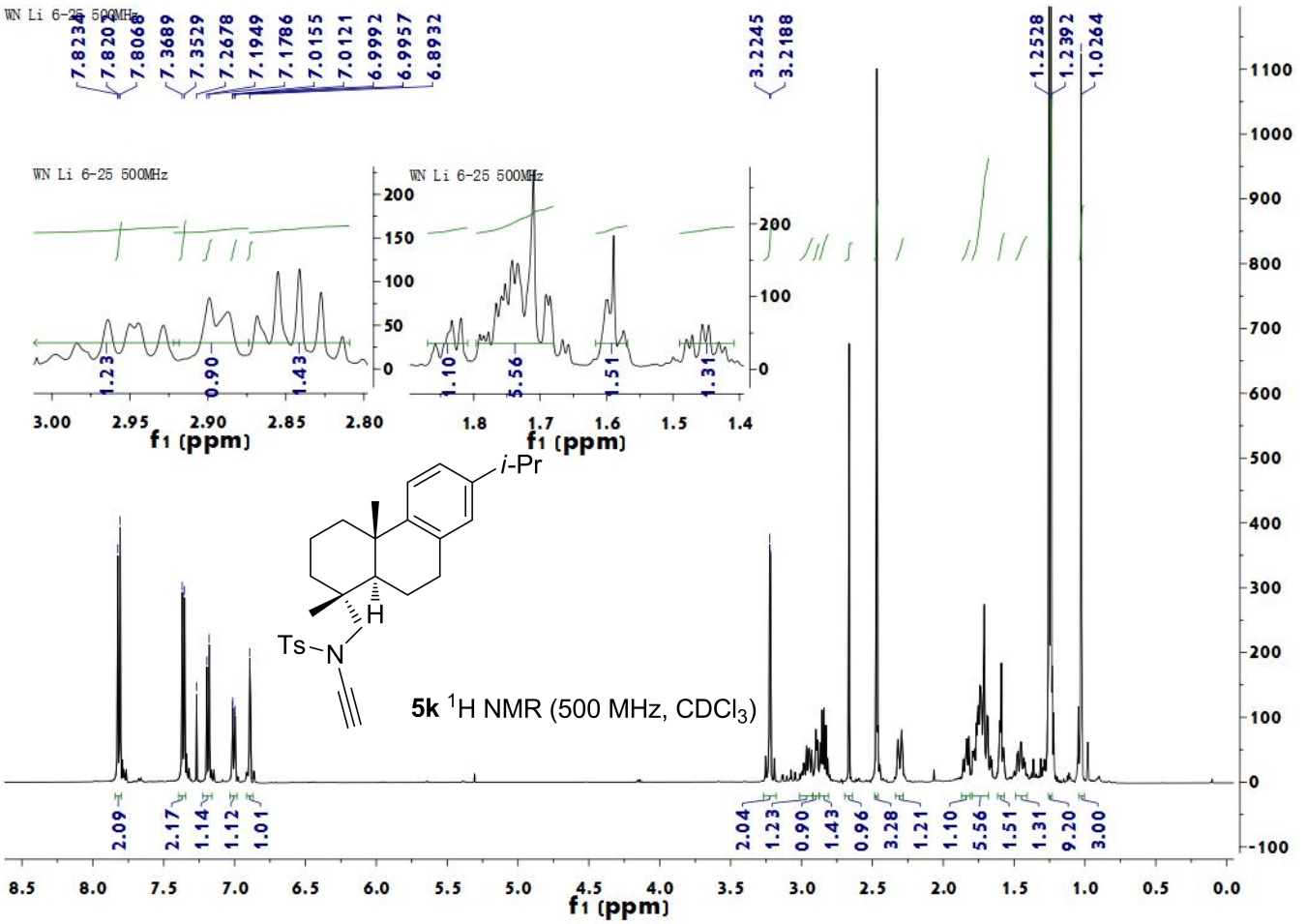




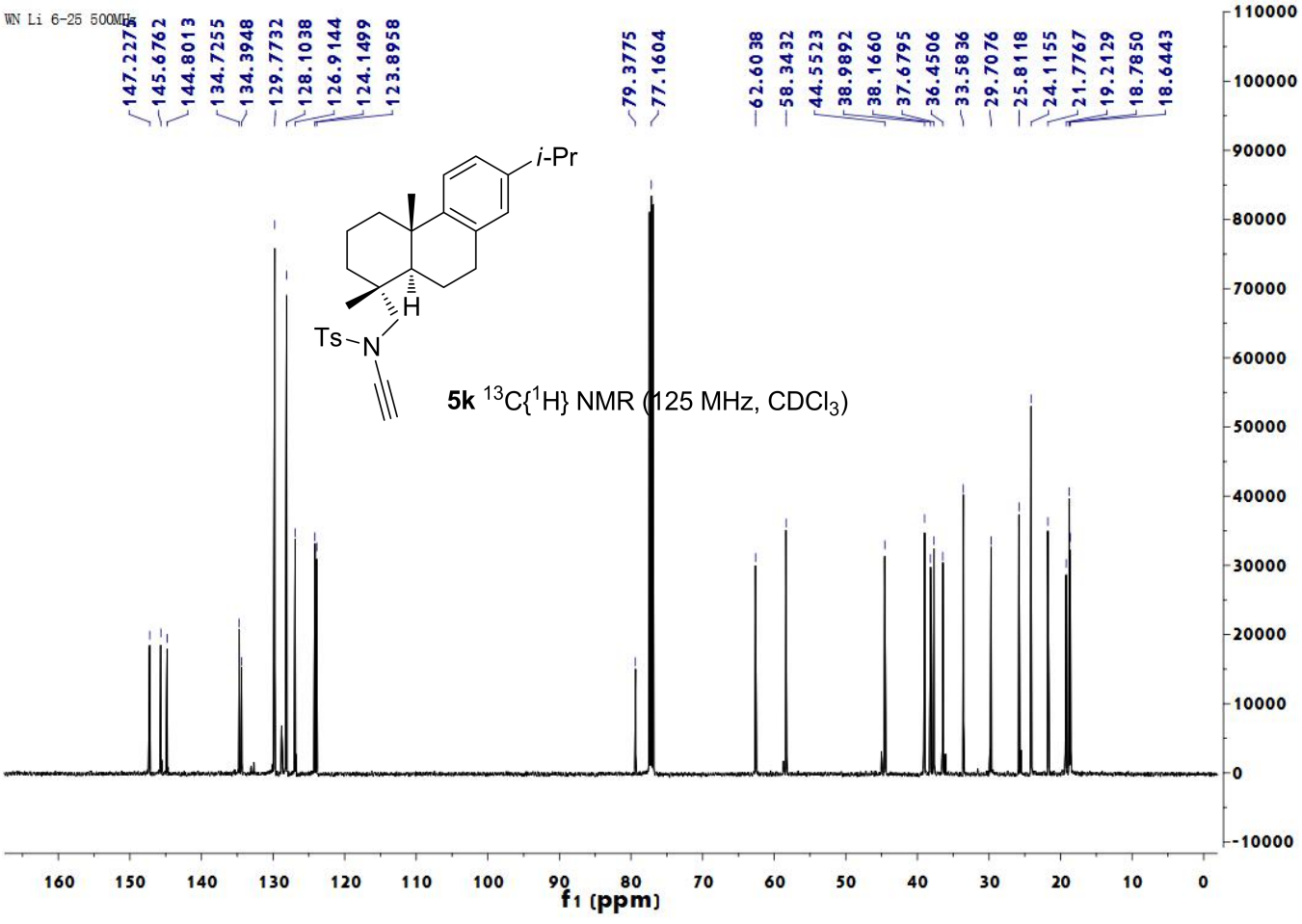

**5j** $^{1}$H NMR (500 MHz, $CDCl_3$)



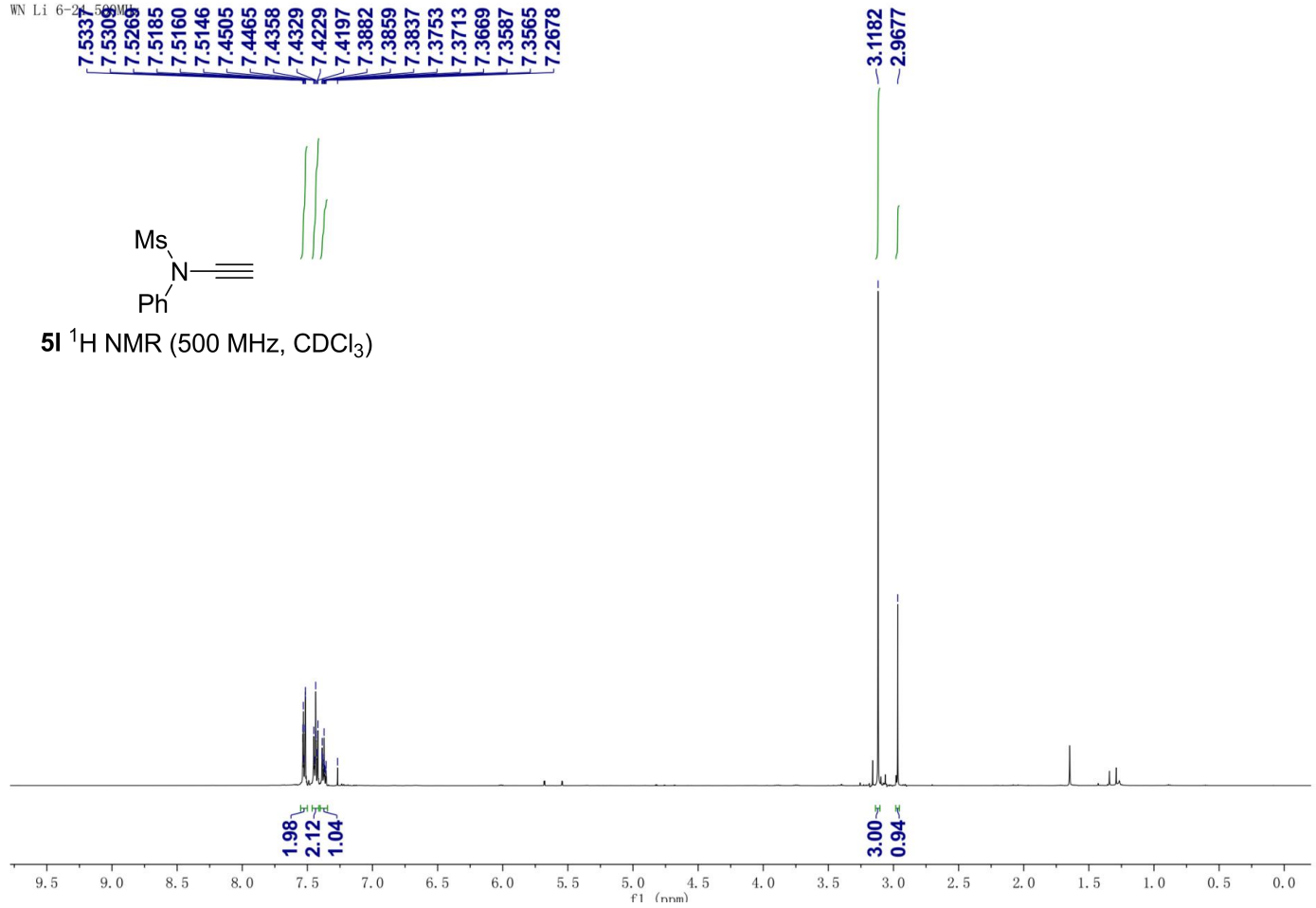

**5j** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



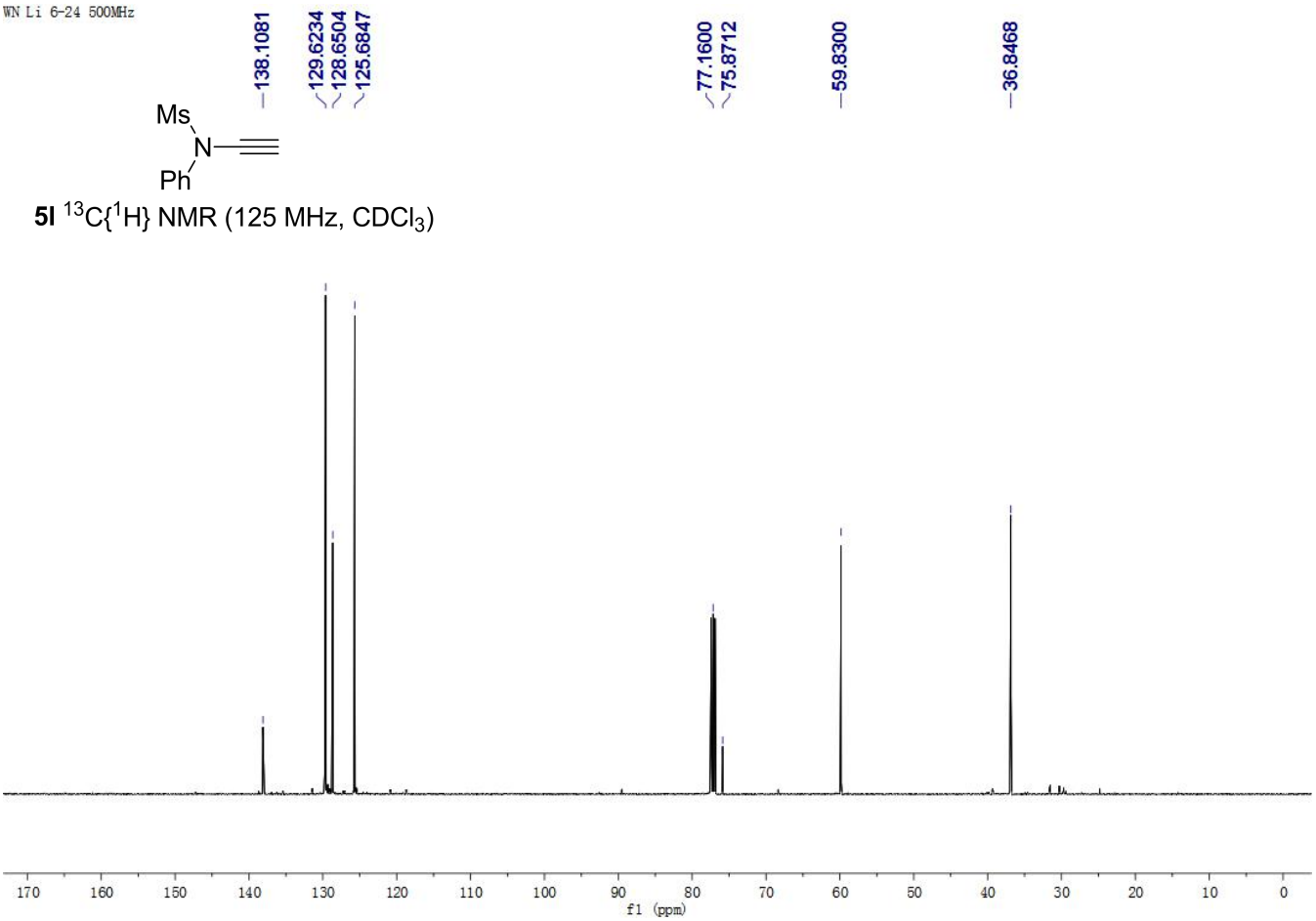

**5k** $^{1}$H NMR (500 MHz, $CDCl_3$)



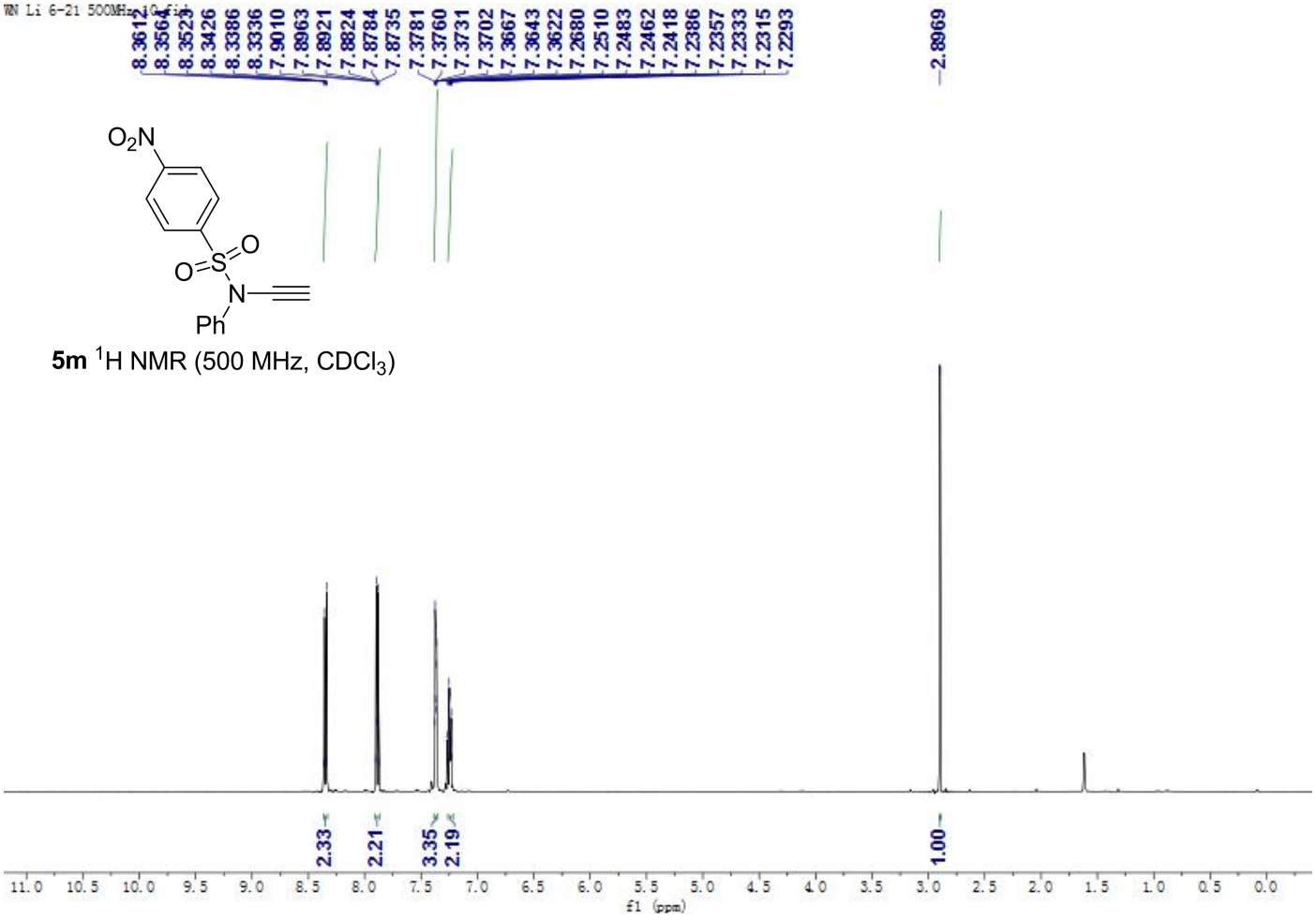

**5k** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



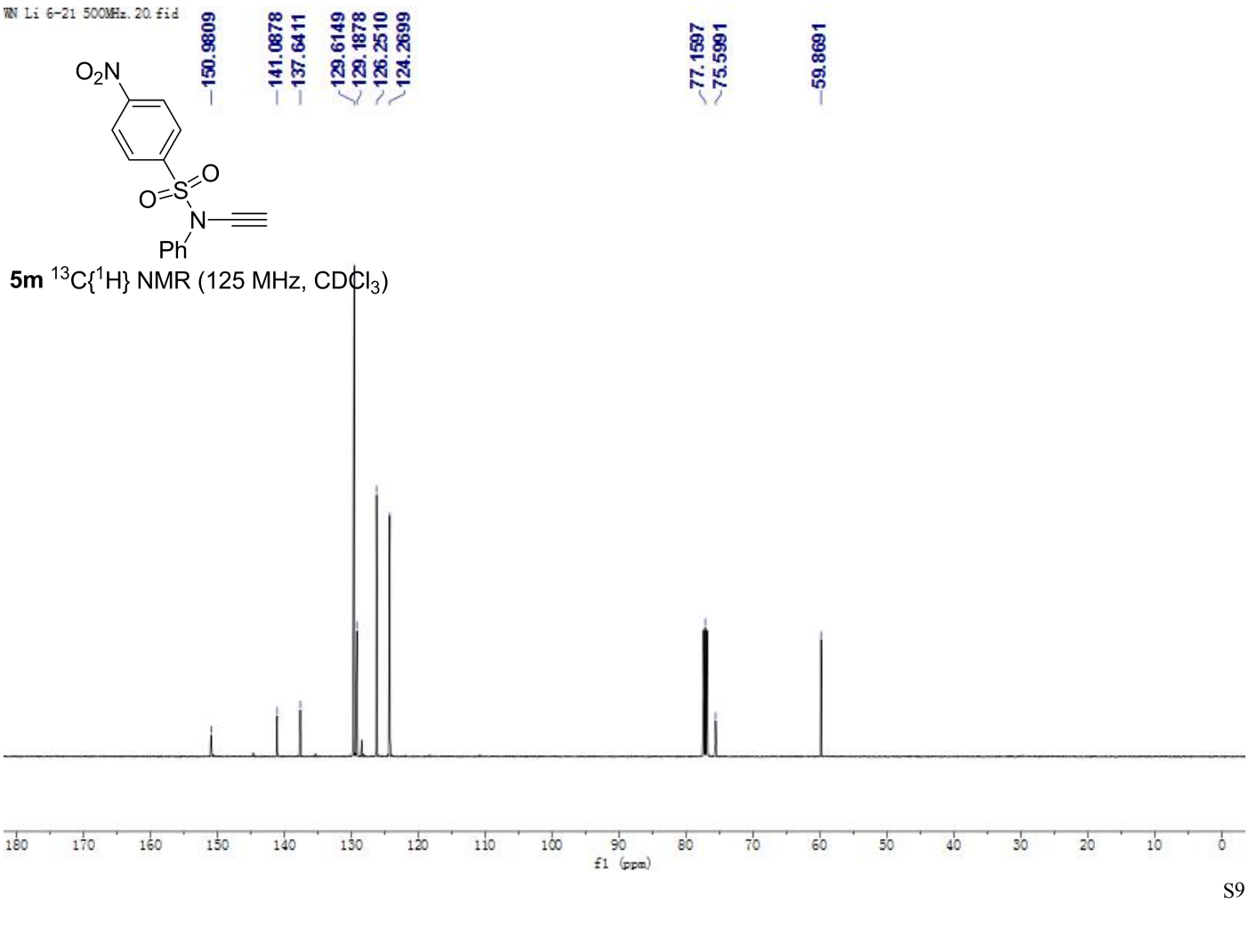

**5l** $^{1}$H NMR (500 MHz, $CDCl_3$)



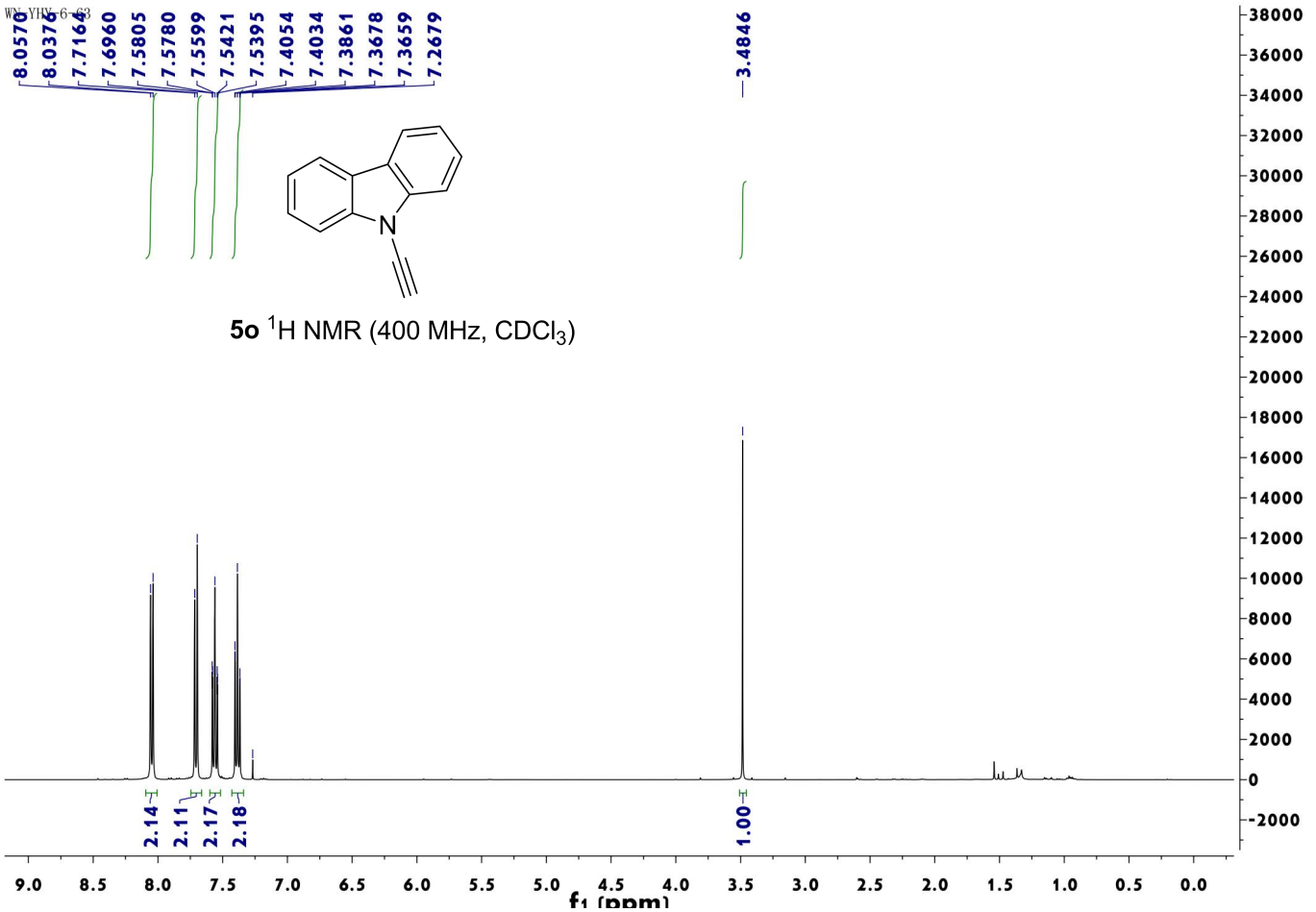

**5l** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



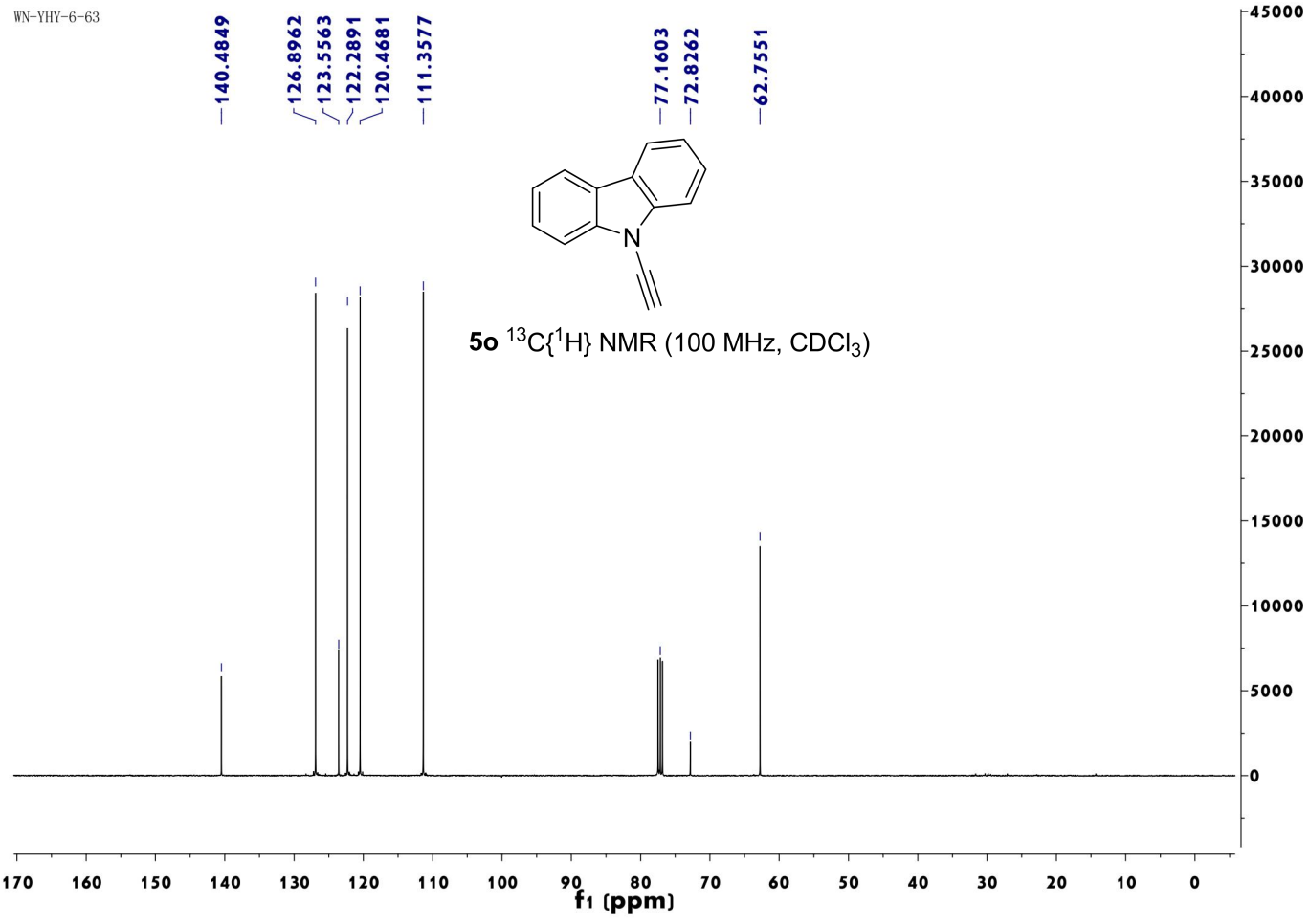

**5m** $^{1}$H NMR (500 MHz, $CDCl_3$)



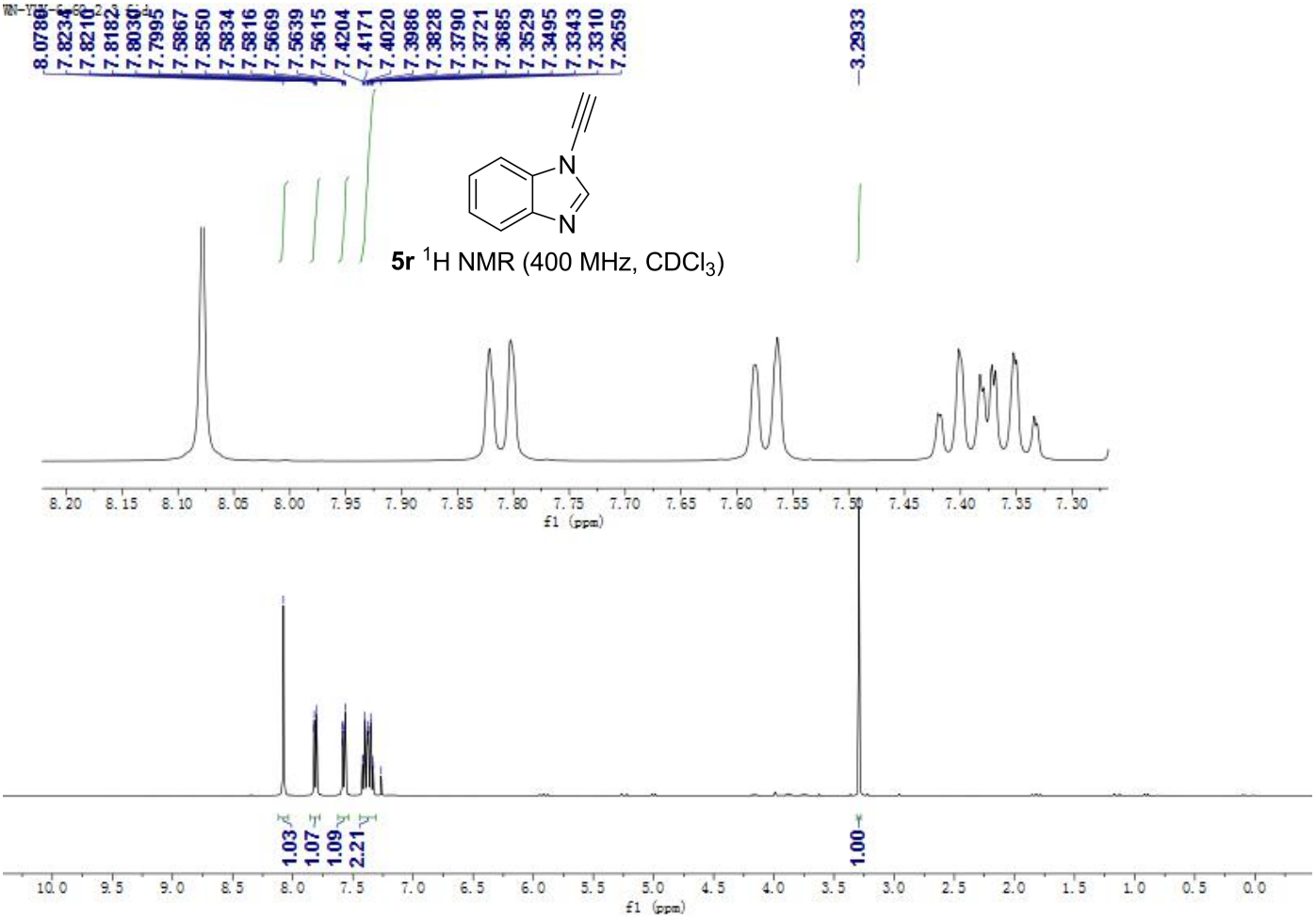

**5m** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



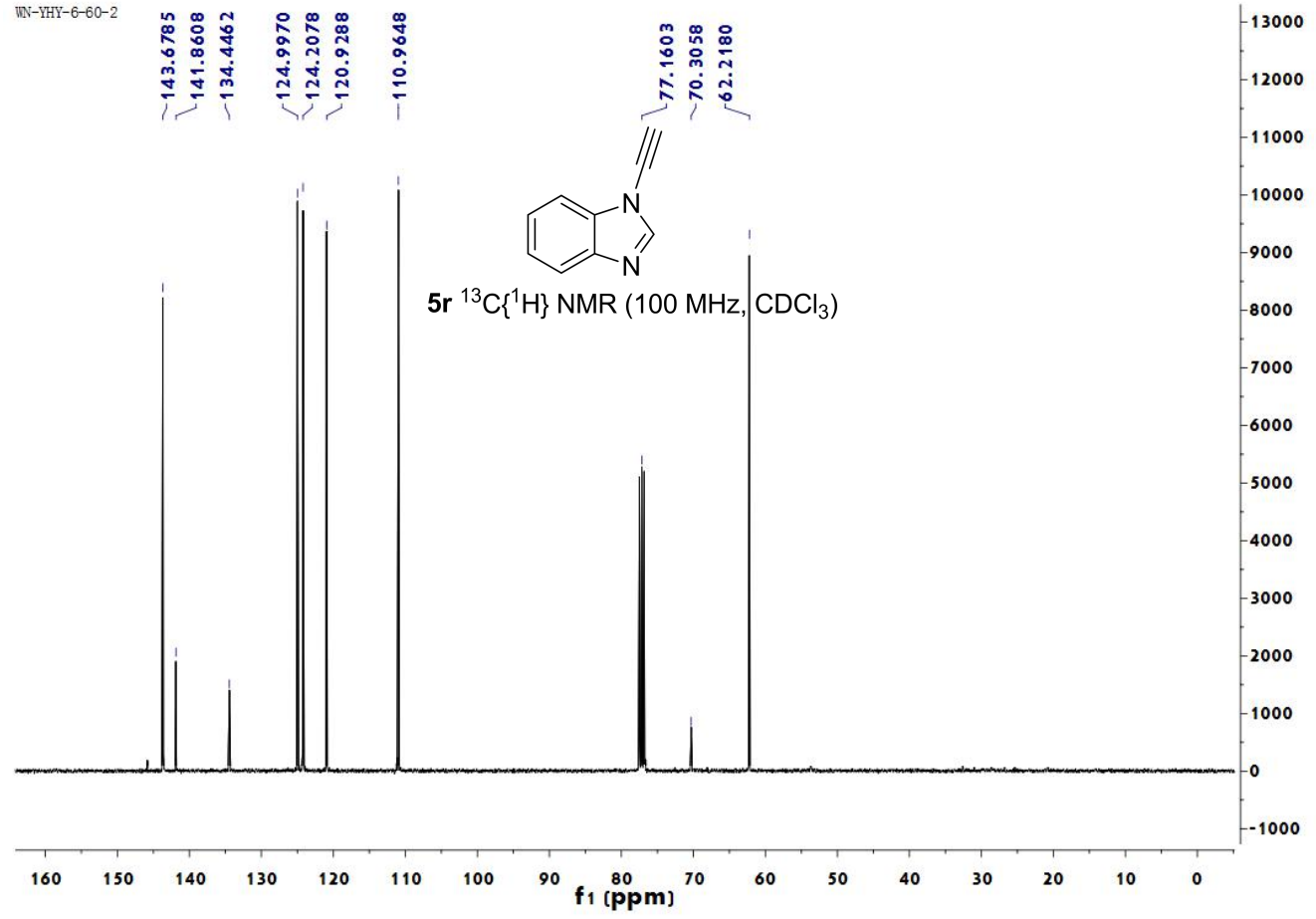

**5o** $^{1}$H NMR (400 MHz, $CDCl_3$)



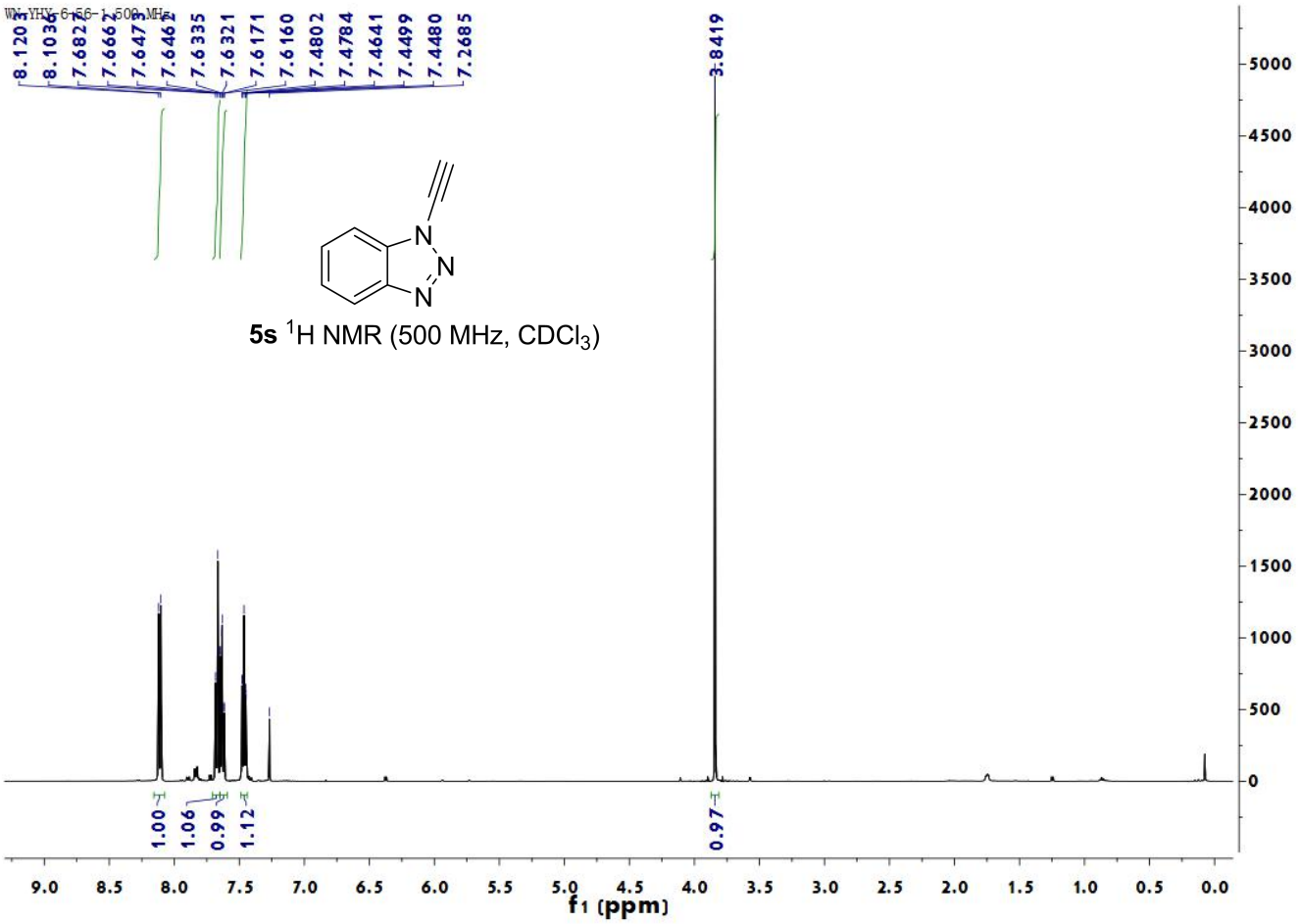

**5o** $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



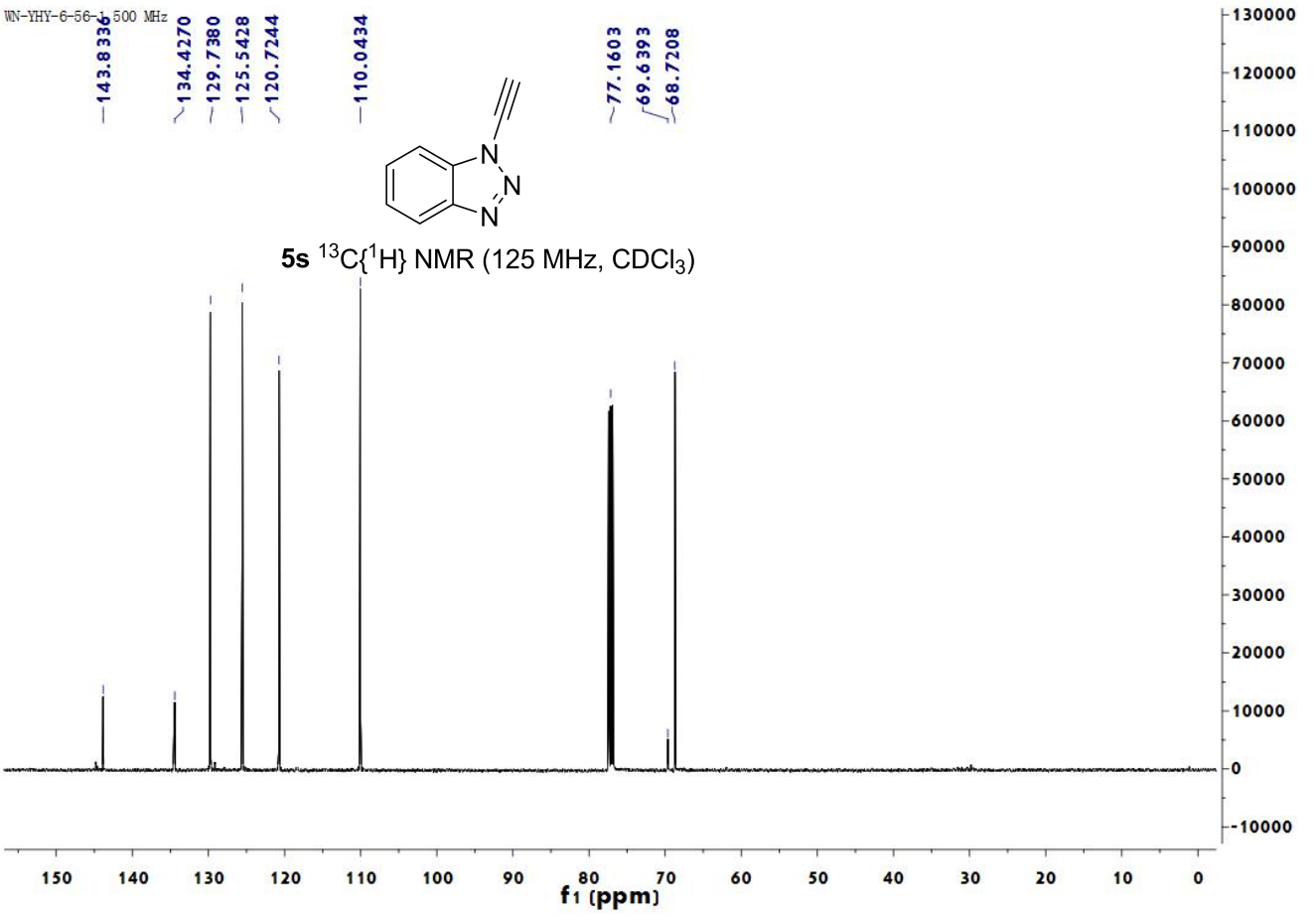

**5r** $^{1}$H NMR (400 MHz, $CDCl_3$)



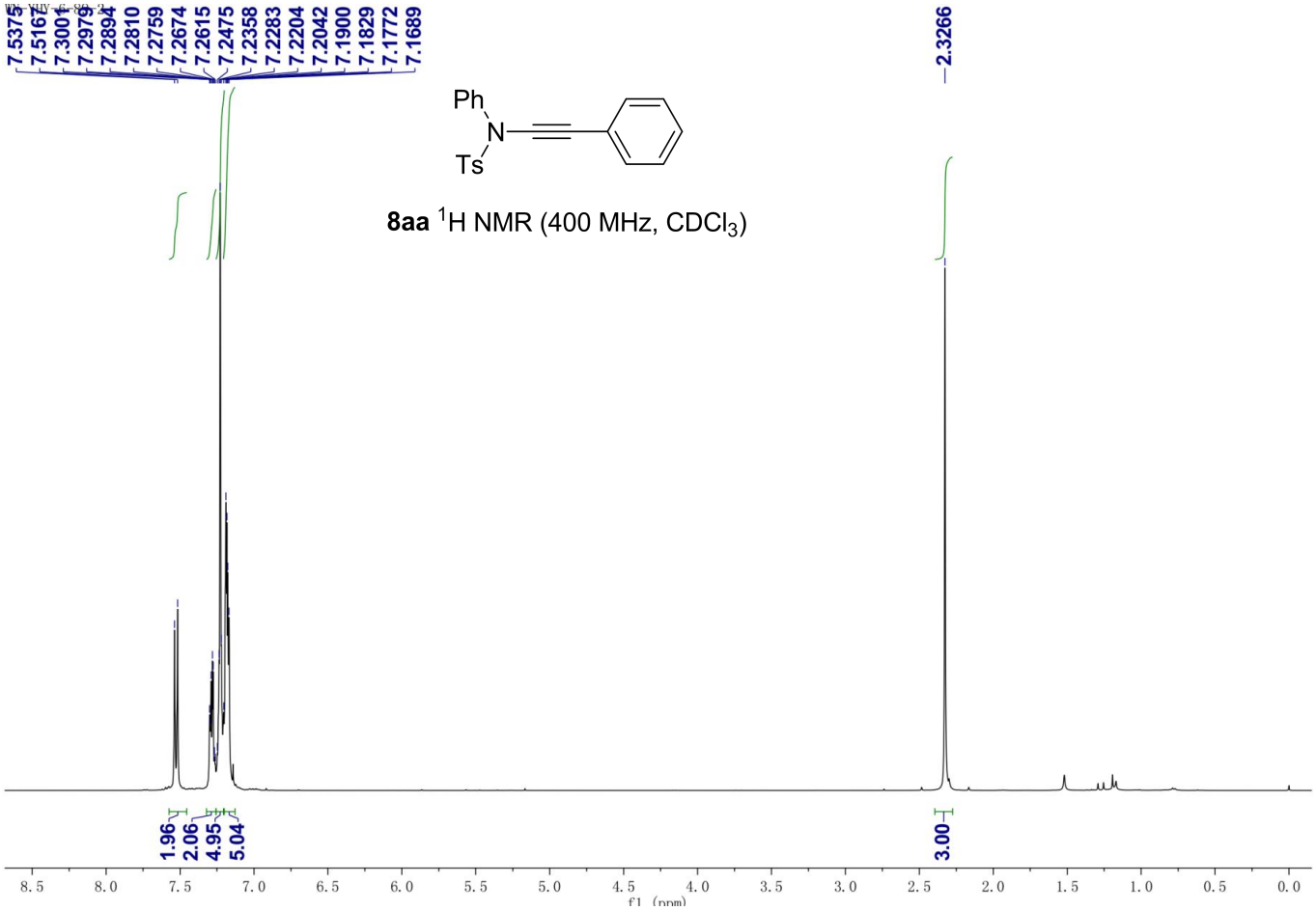

**5r** $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



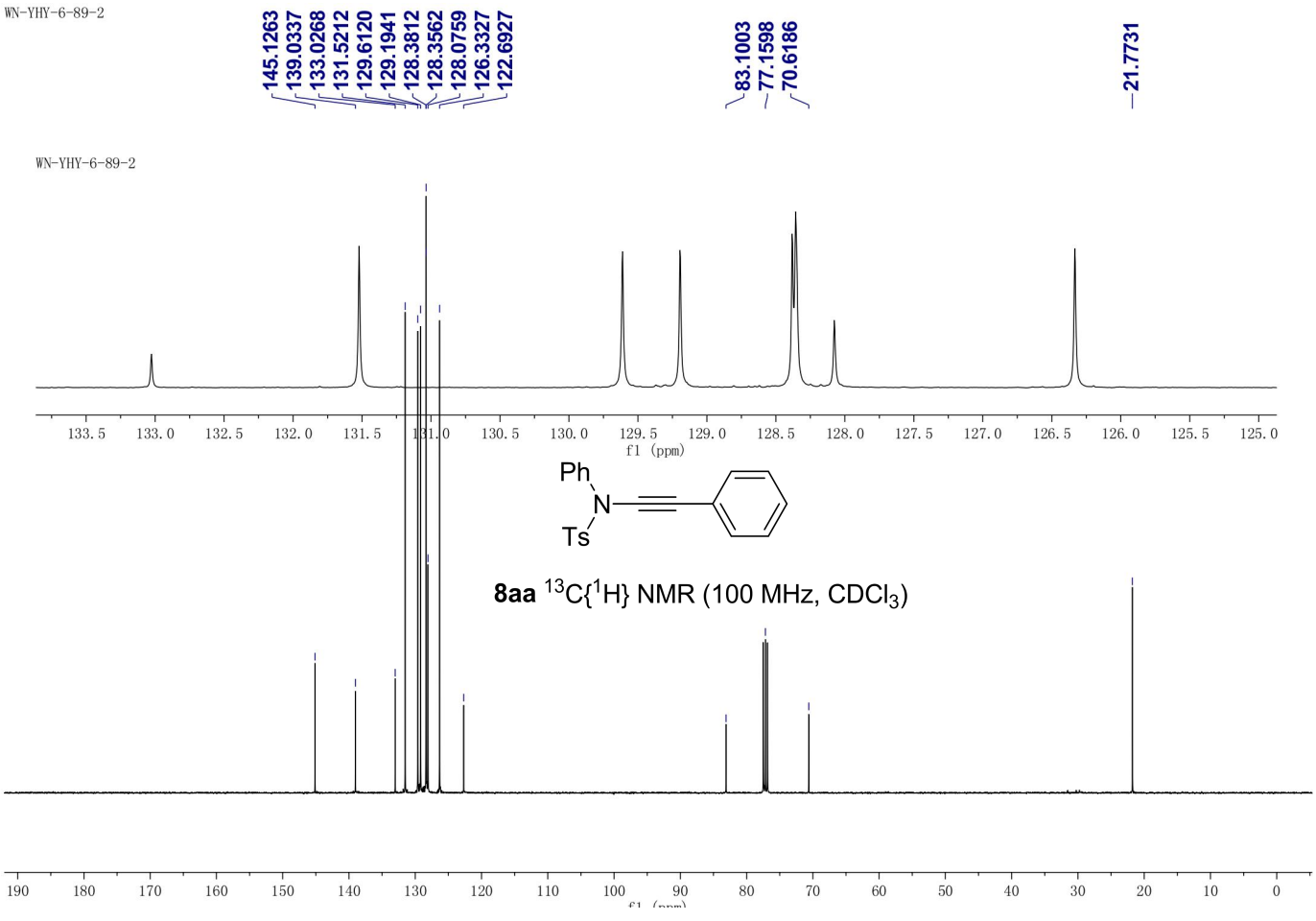

**5s** $^{1}$H NMR (500 MHz, $CDCl_3$)



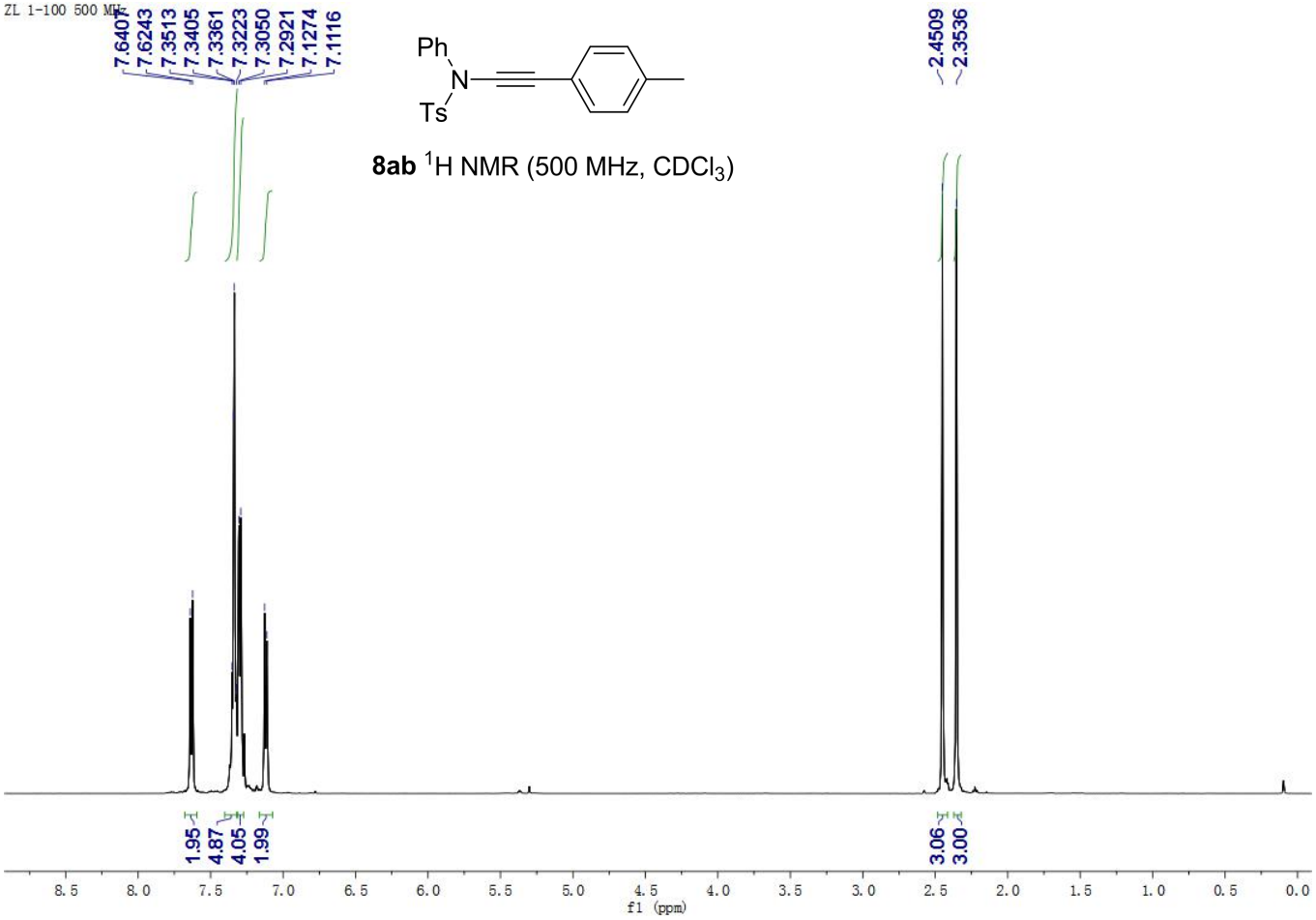

**5s** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



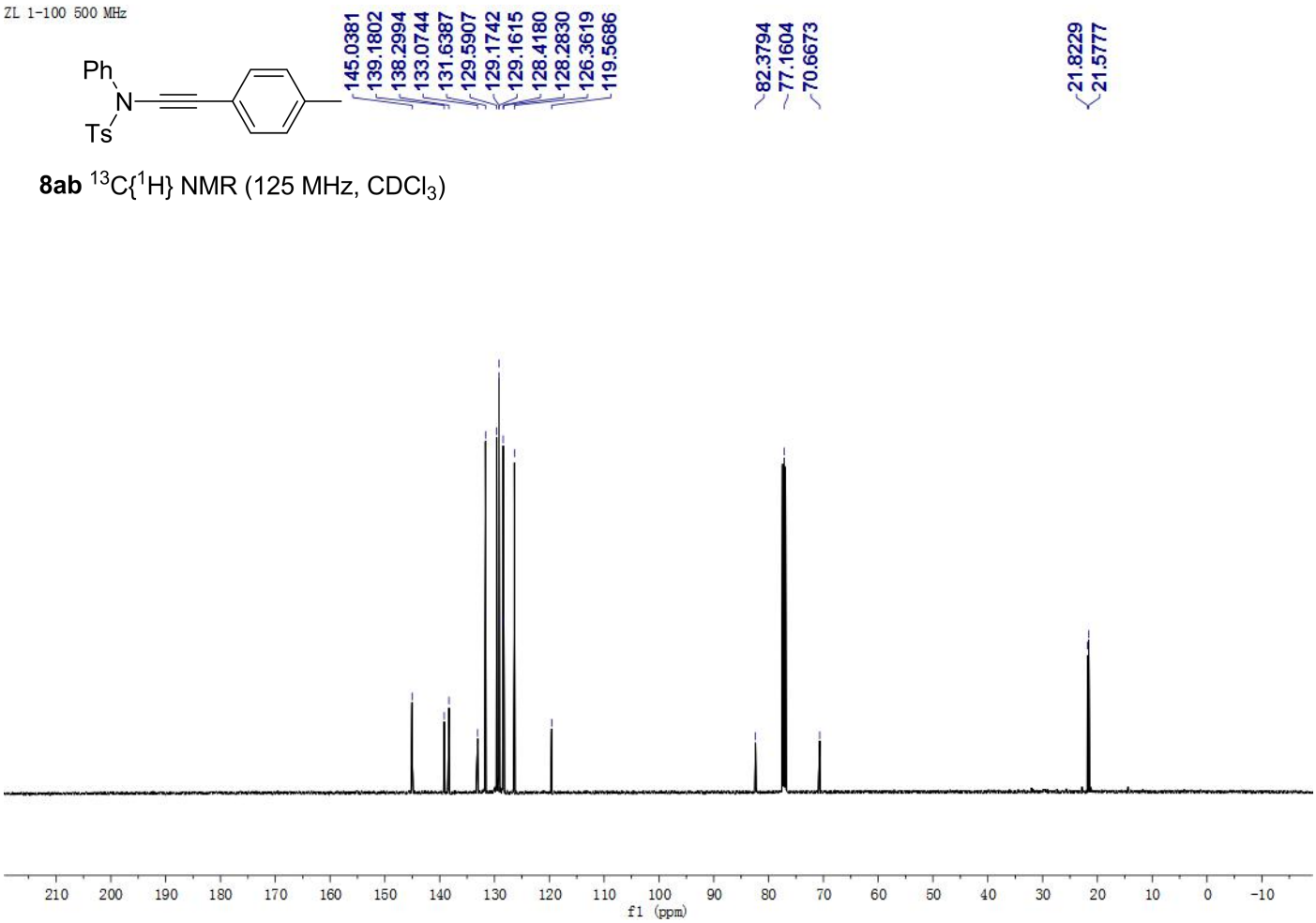

**8aa** $^{1}$H NMR (400 MHz, $CDCl_3$)



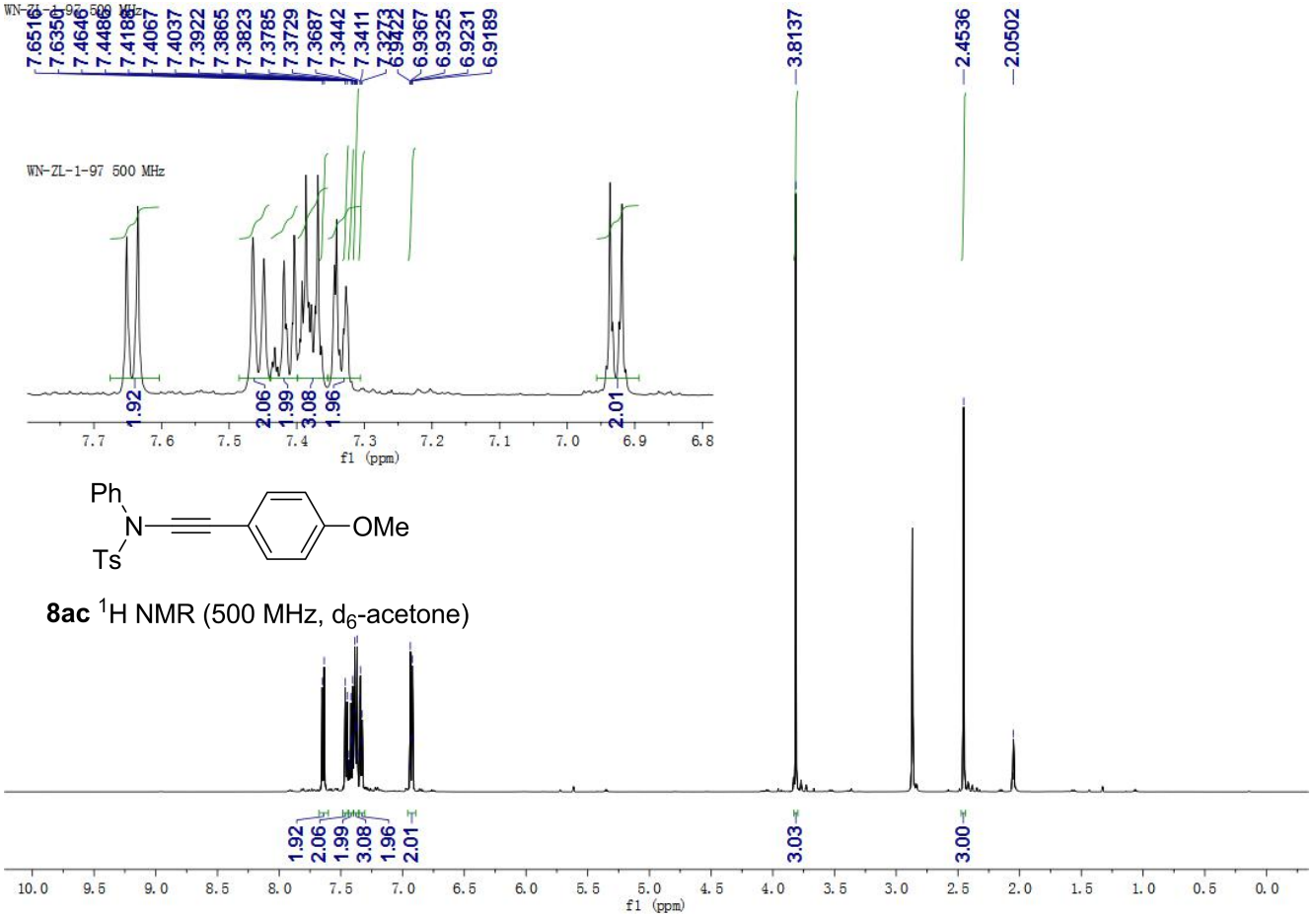

**8aa** $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



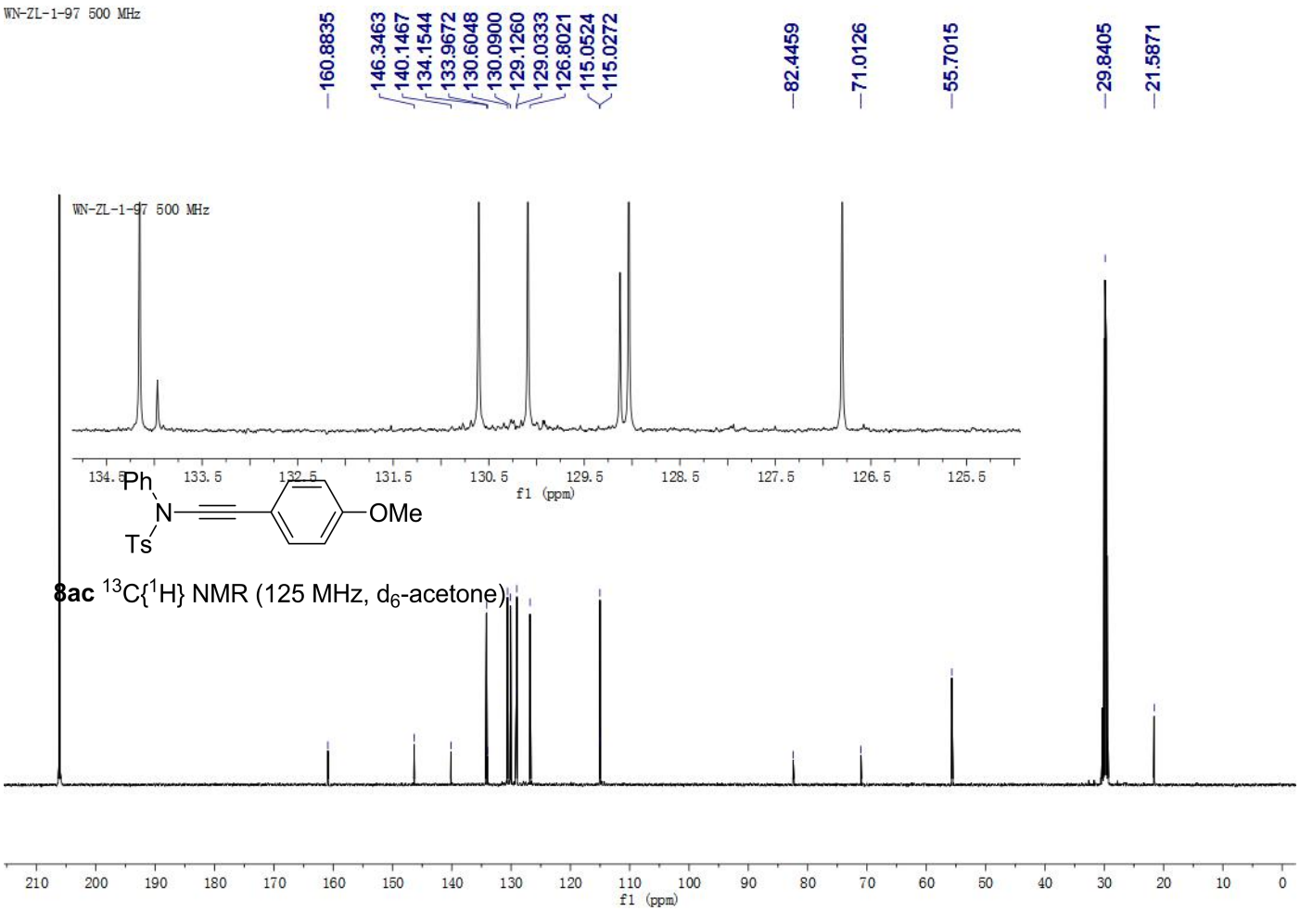

**8ab** $^{1}$H NMR (500 MHz, $CDCl_3$)



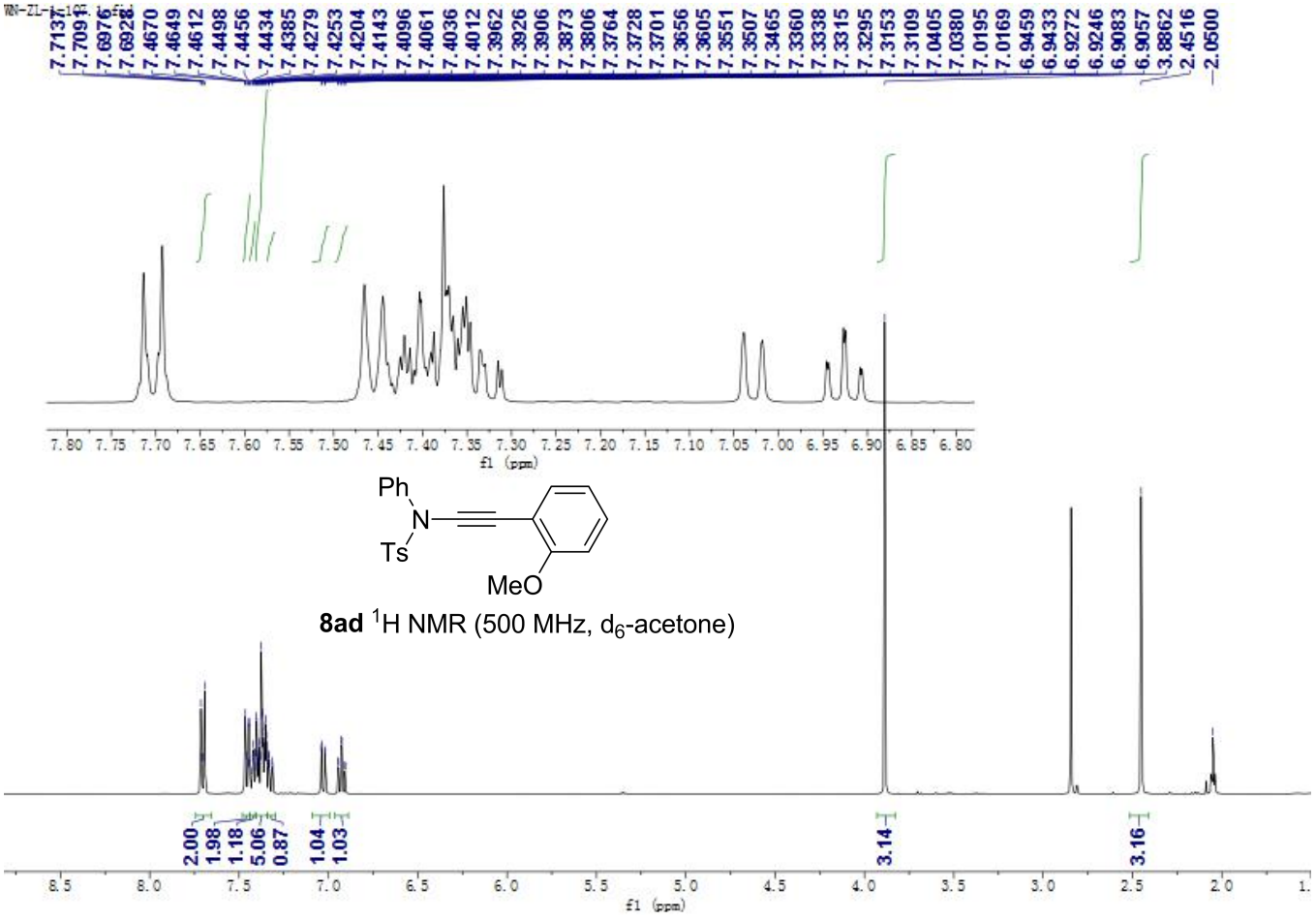

**8ab** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



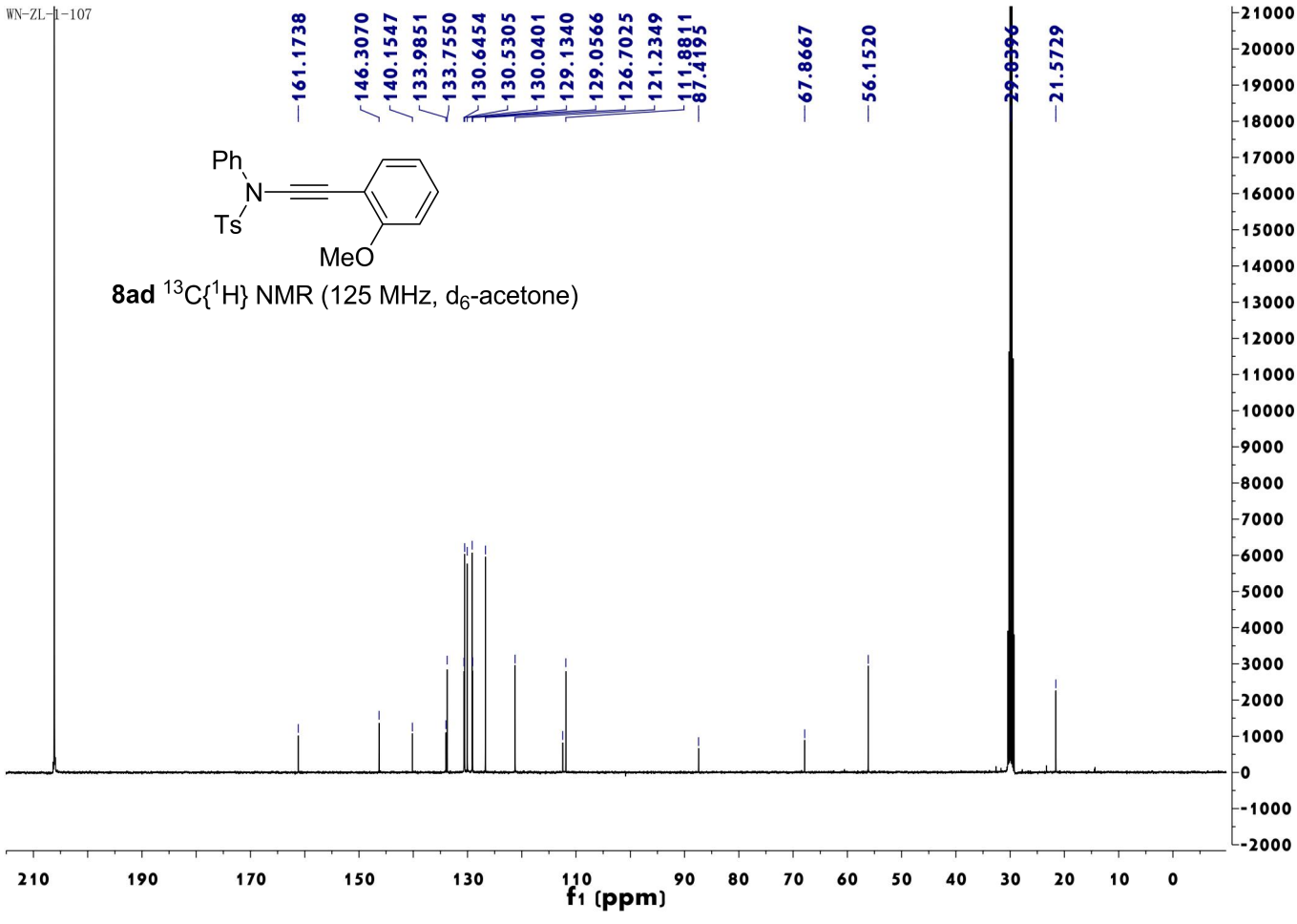

**8ac** $^{1}$H NMR (500 MHz, $d_6$-acetone)



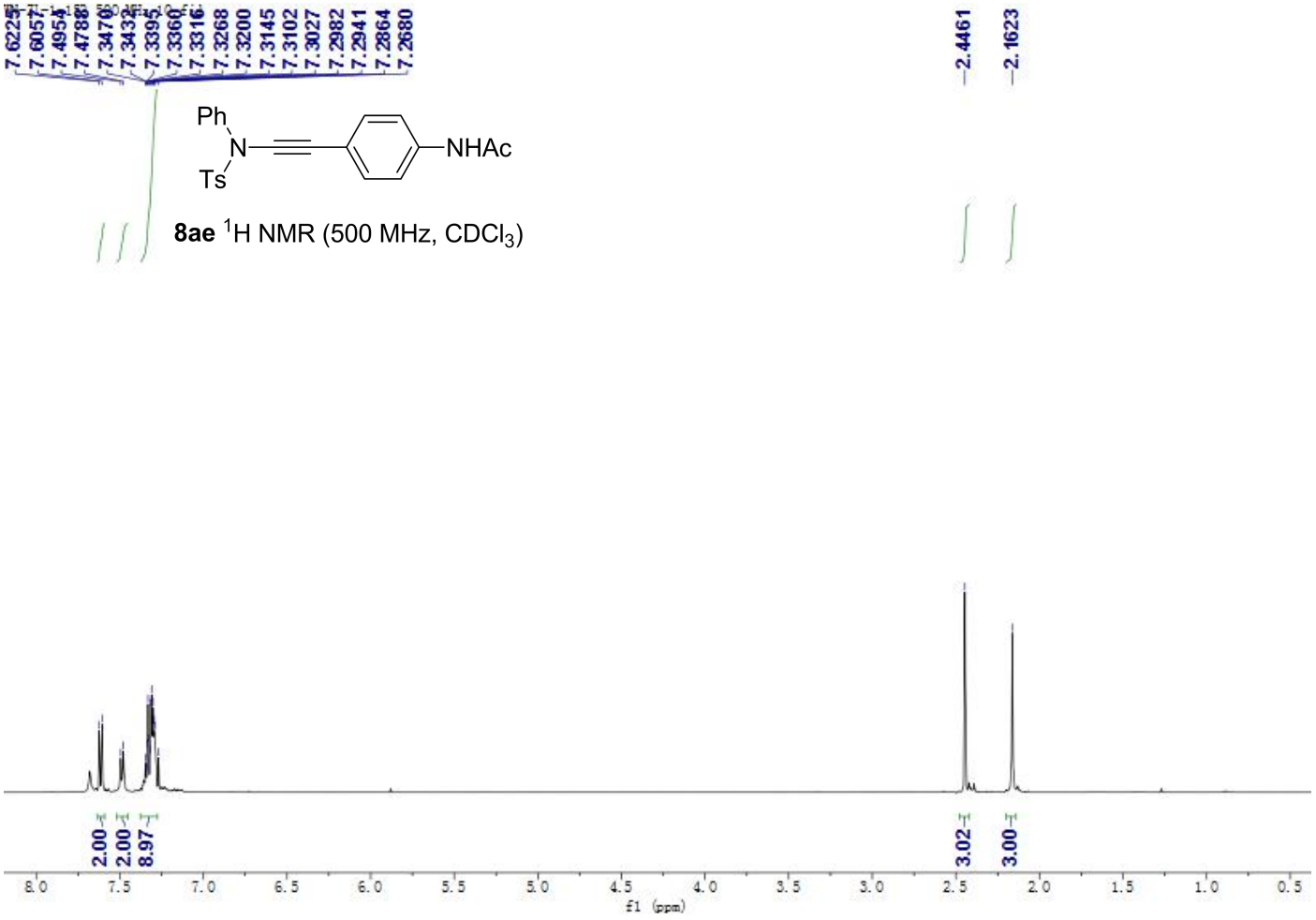

**8ac** $^{13}$C{$^{1}$H} NMR (125 MHz, $d_6$-acetone)



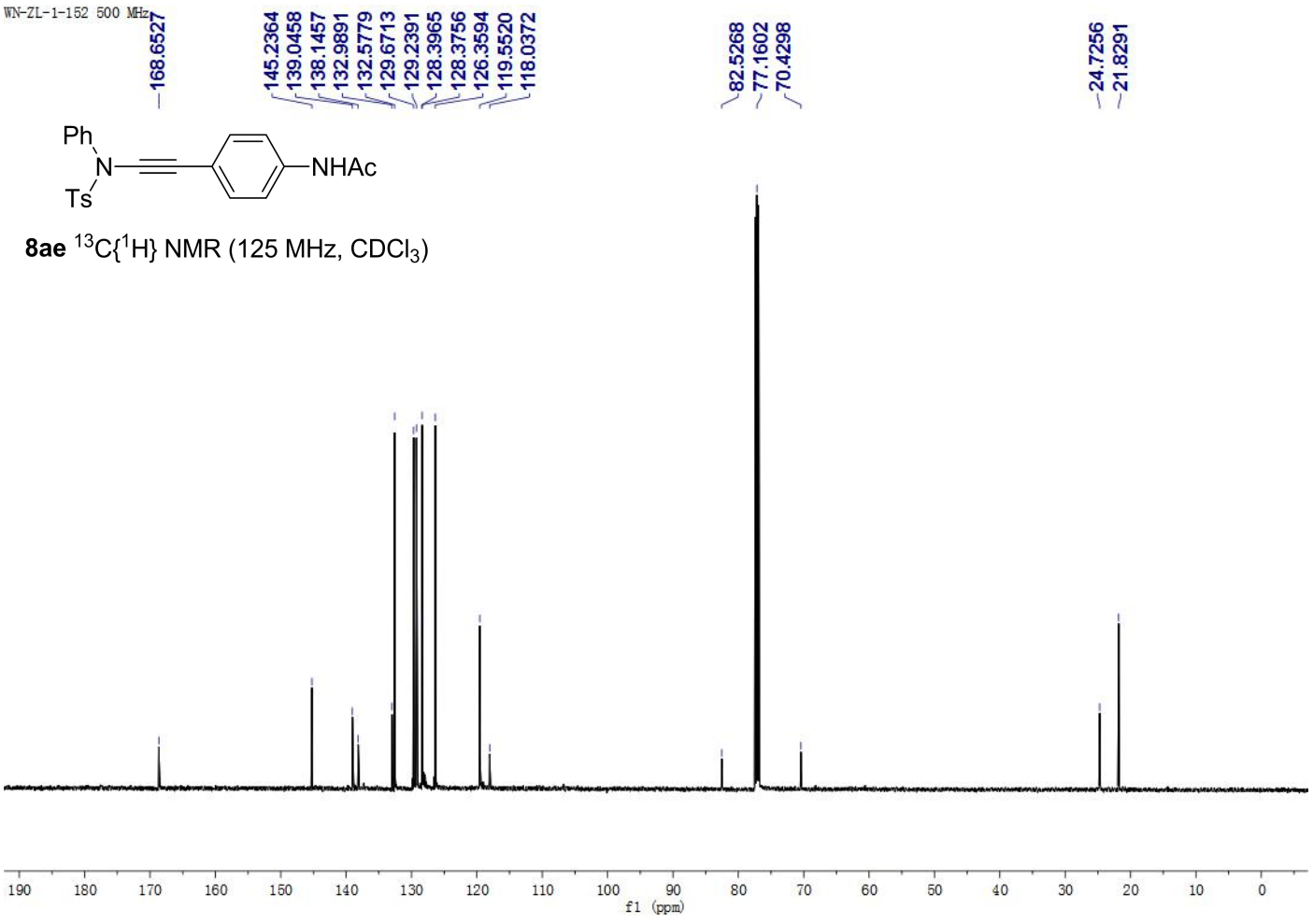

**8ad** $^{1}$H NMR (500 MHz, $d_6$-acetone)



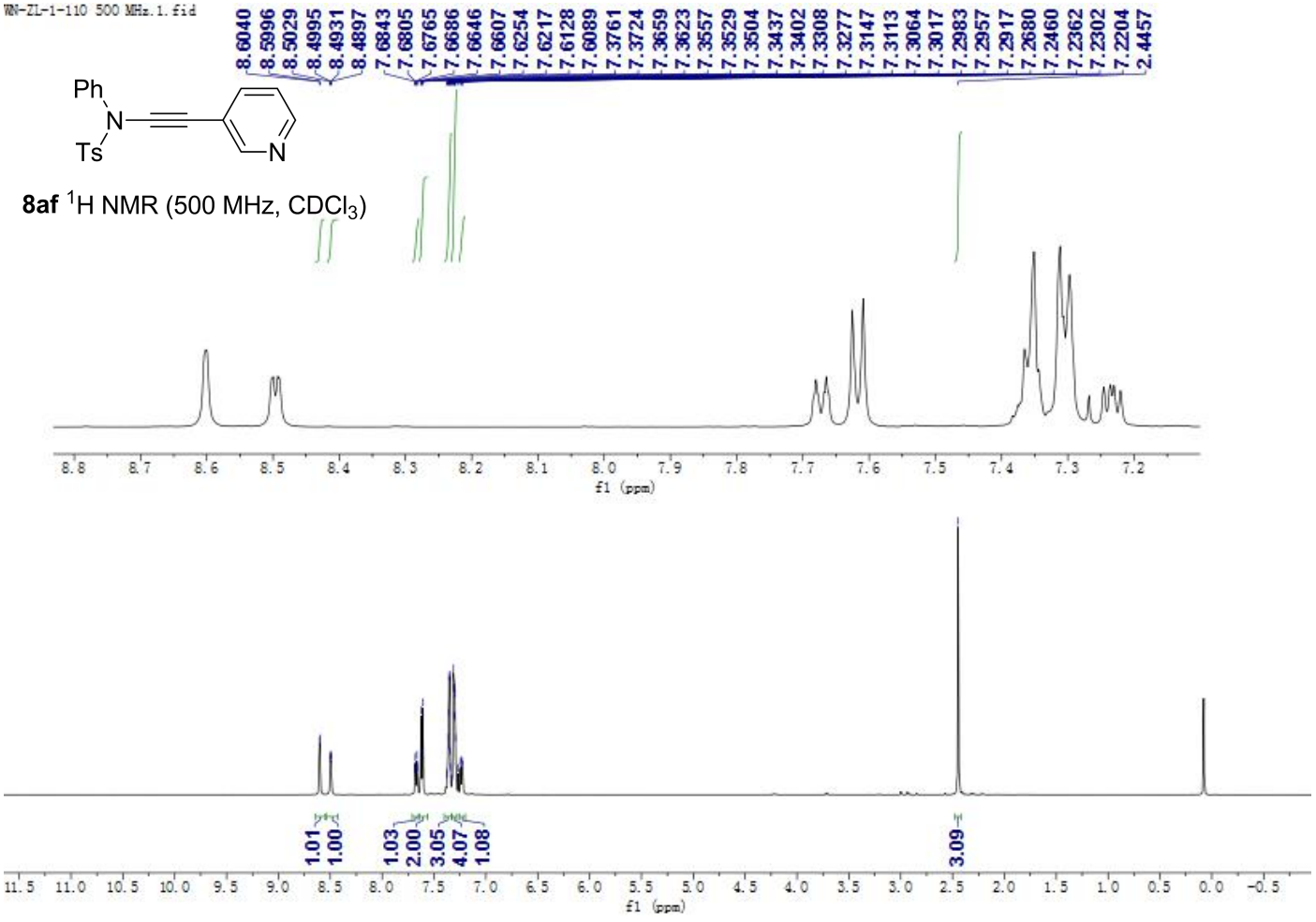

**8ad** $^{13}C\{^{1}H\}$ NMR (125 MHz, $d_6$-acetone)



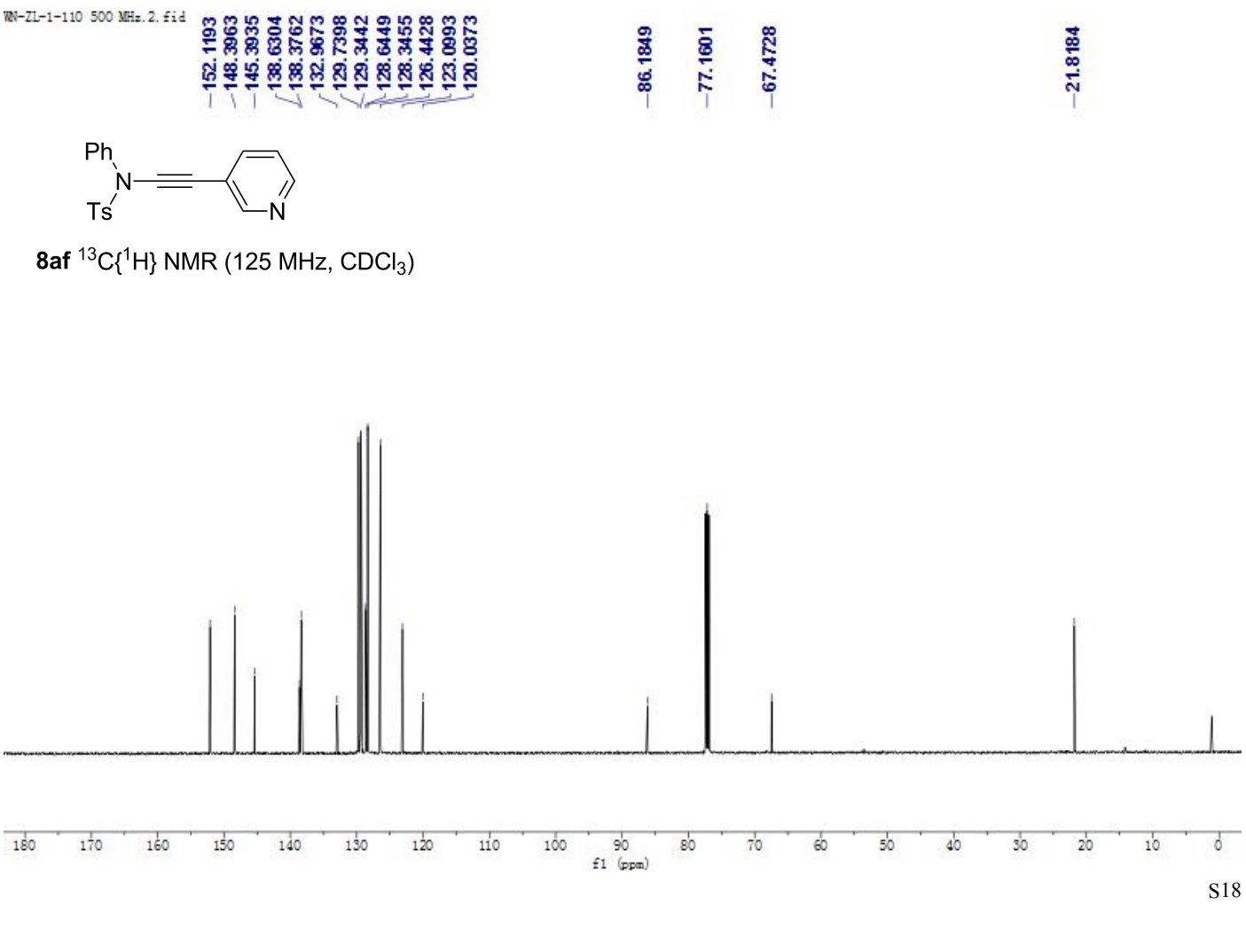

**8ae** $^{1}$H NMR (500 MHz, $CDCl_3$)



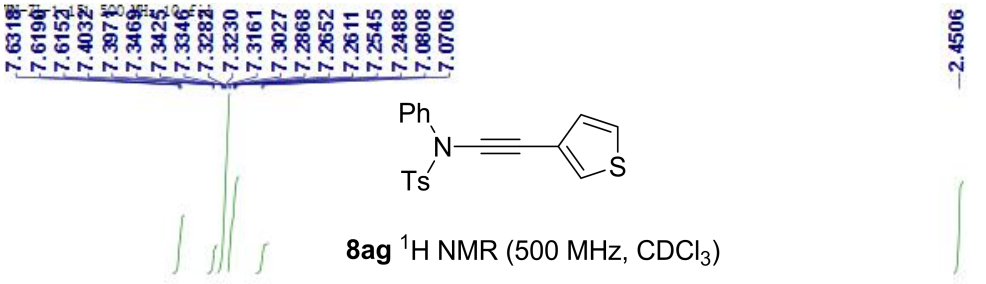

**8ae** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



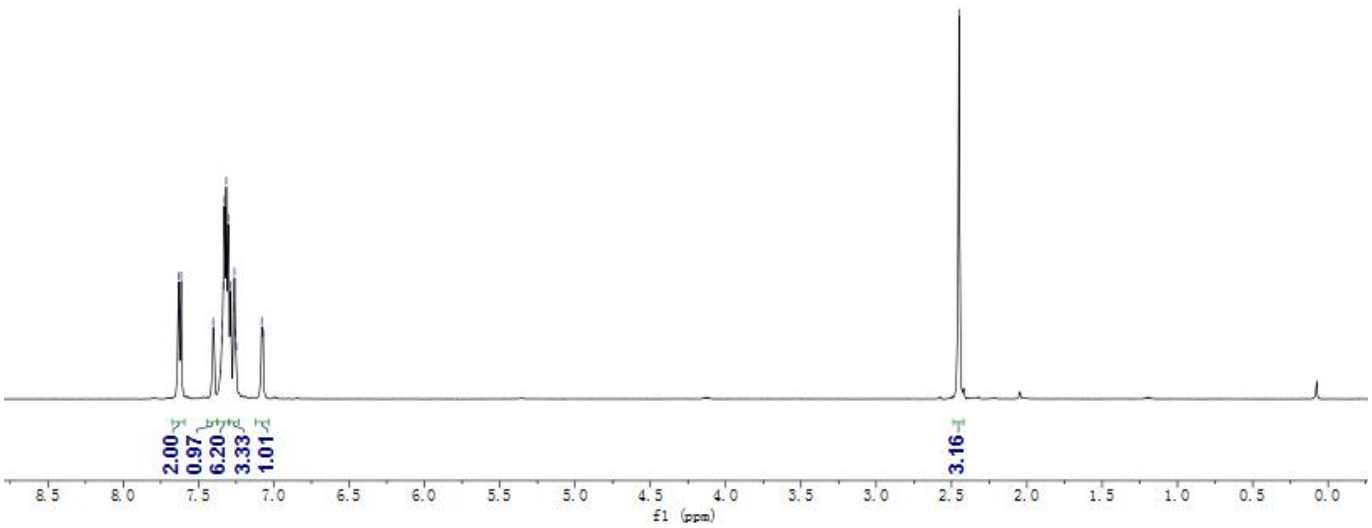

**8af** $^{1}$H NMR (500 MHz, $CDCl_3$)

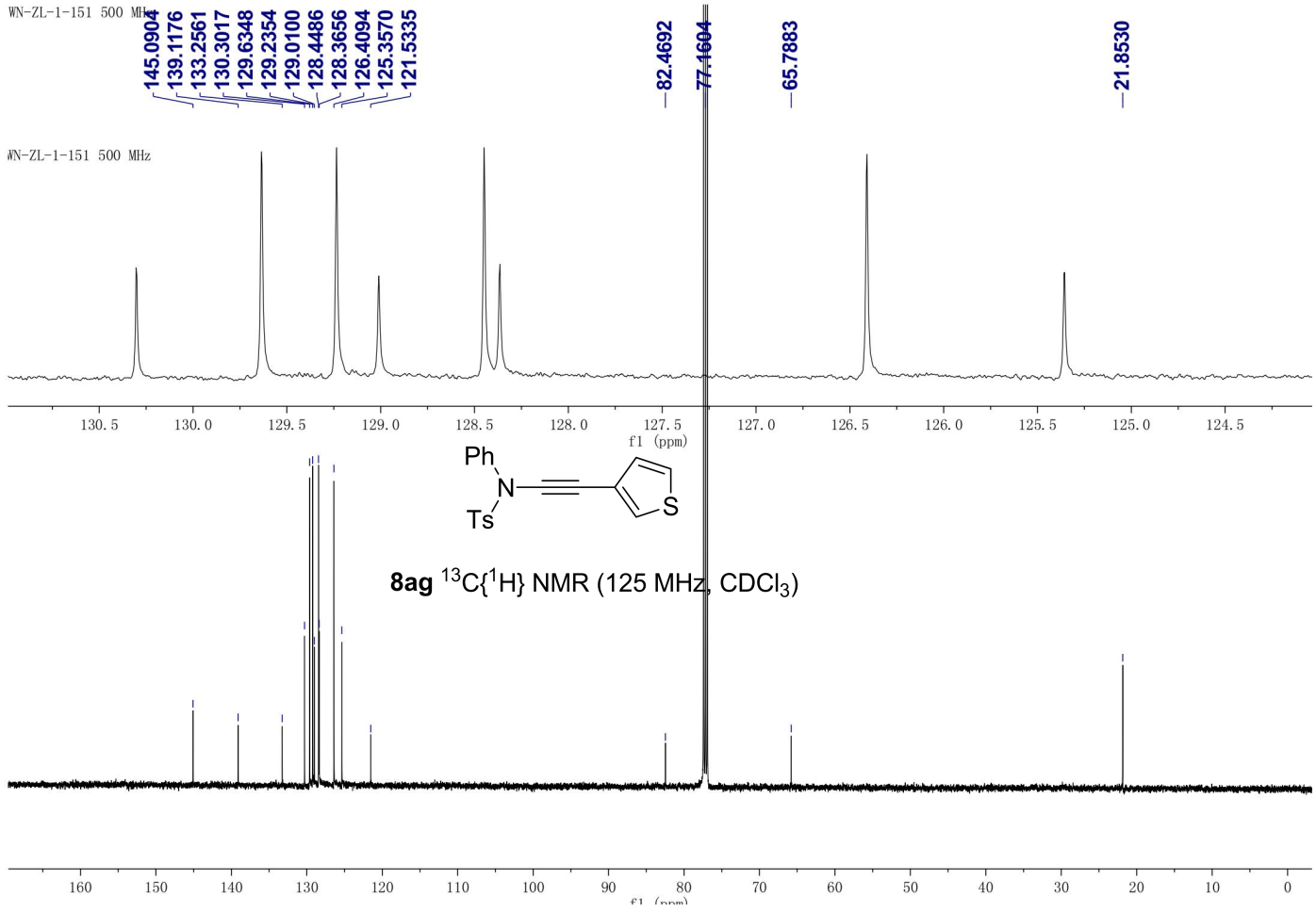



**8af** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)




**8ag** $^{1}$H NMR (500 MHz, $CDCl_3$)

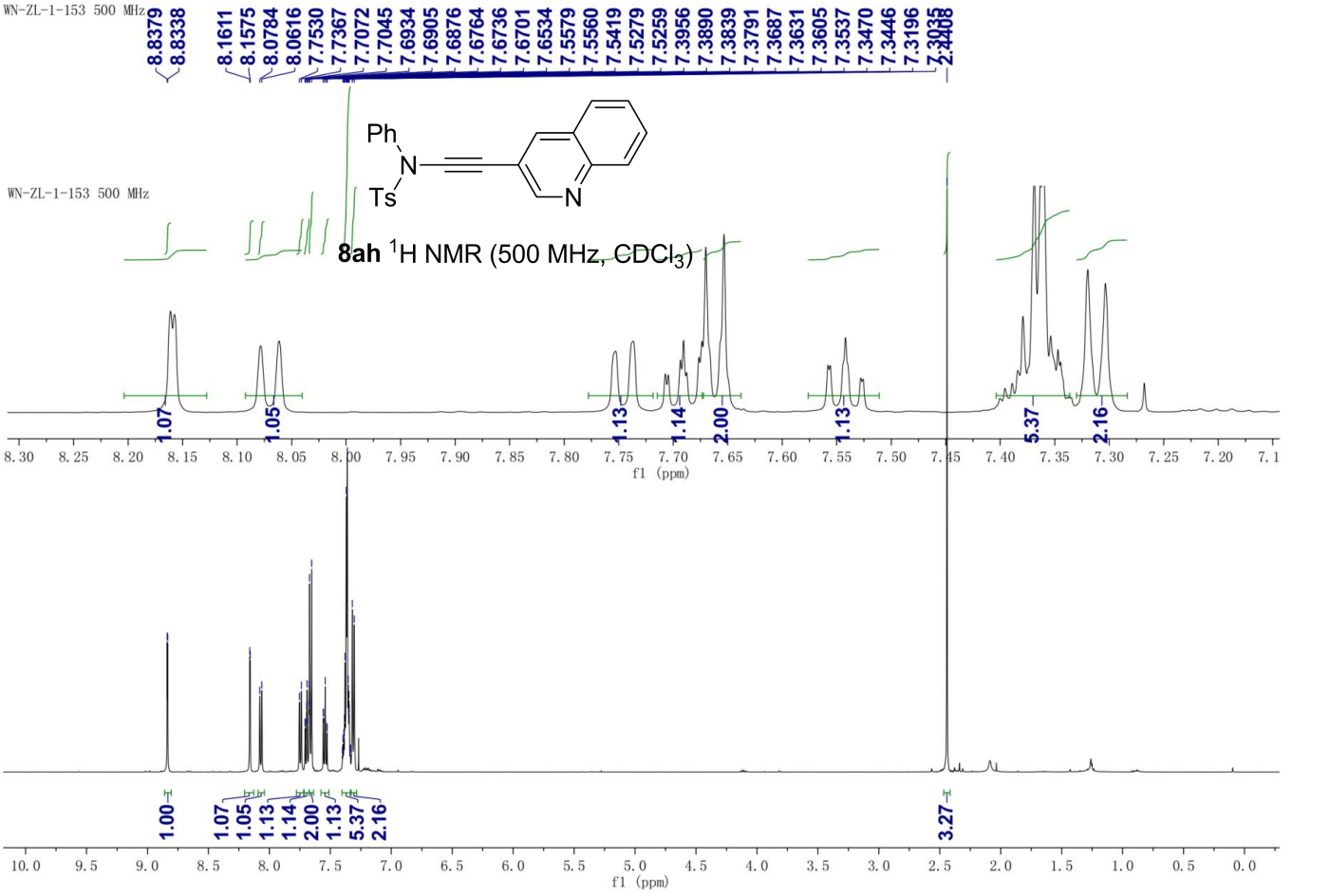


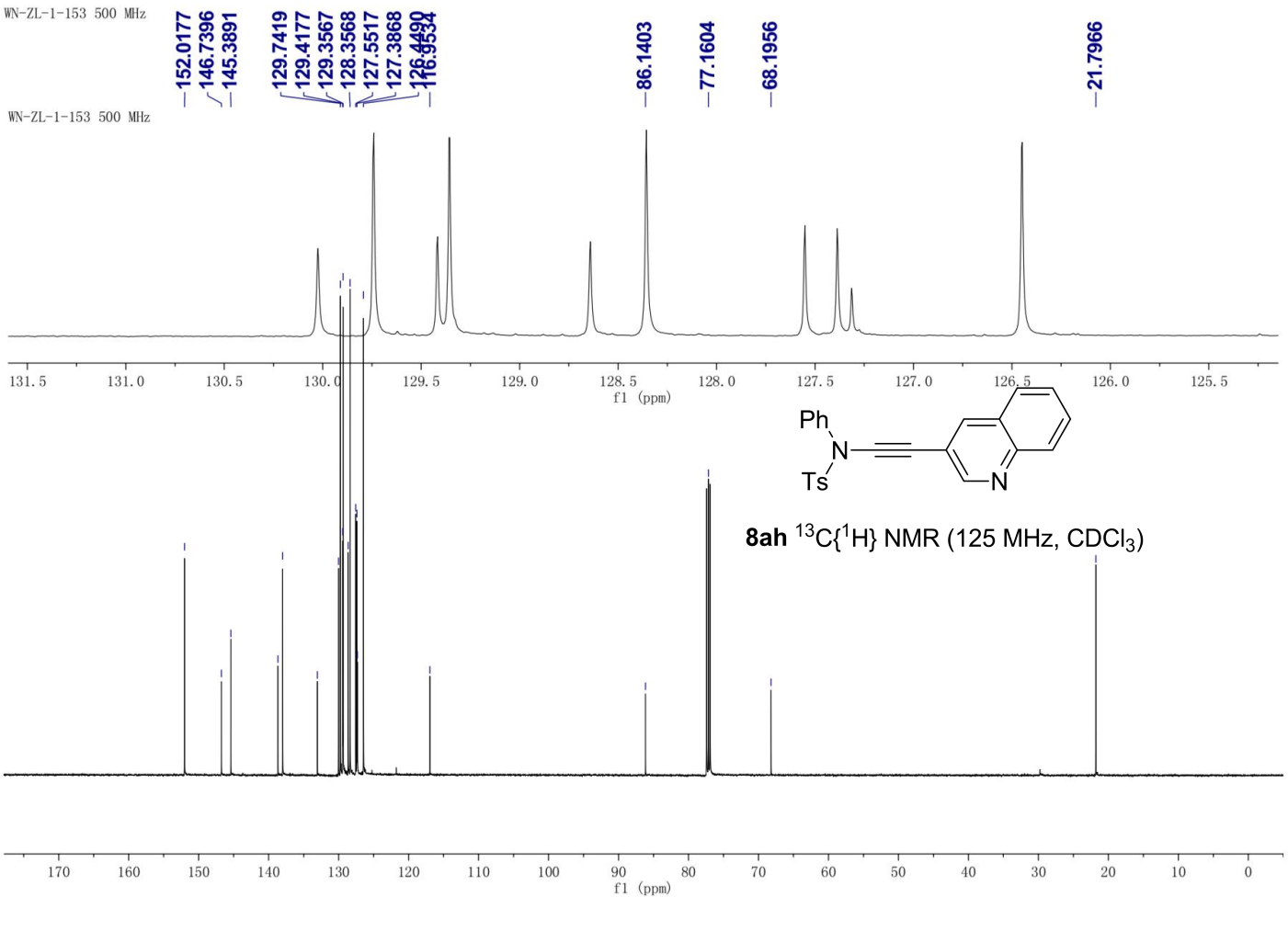




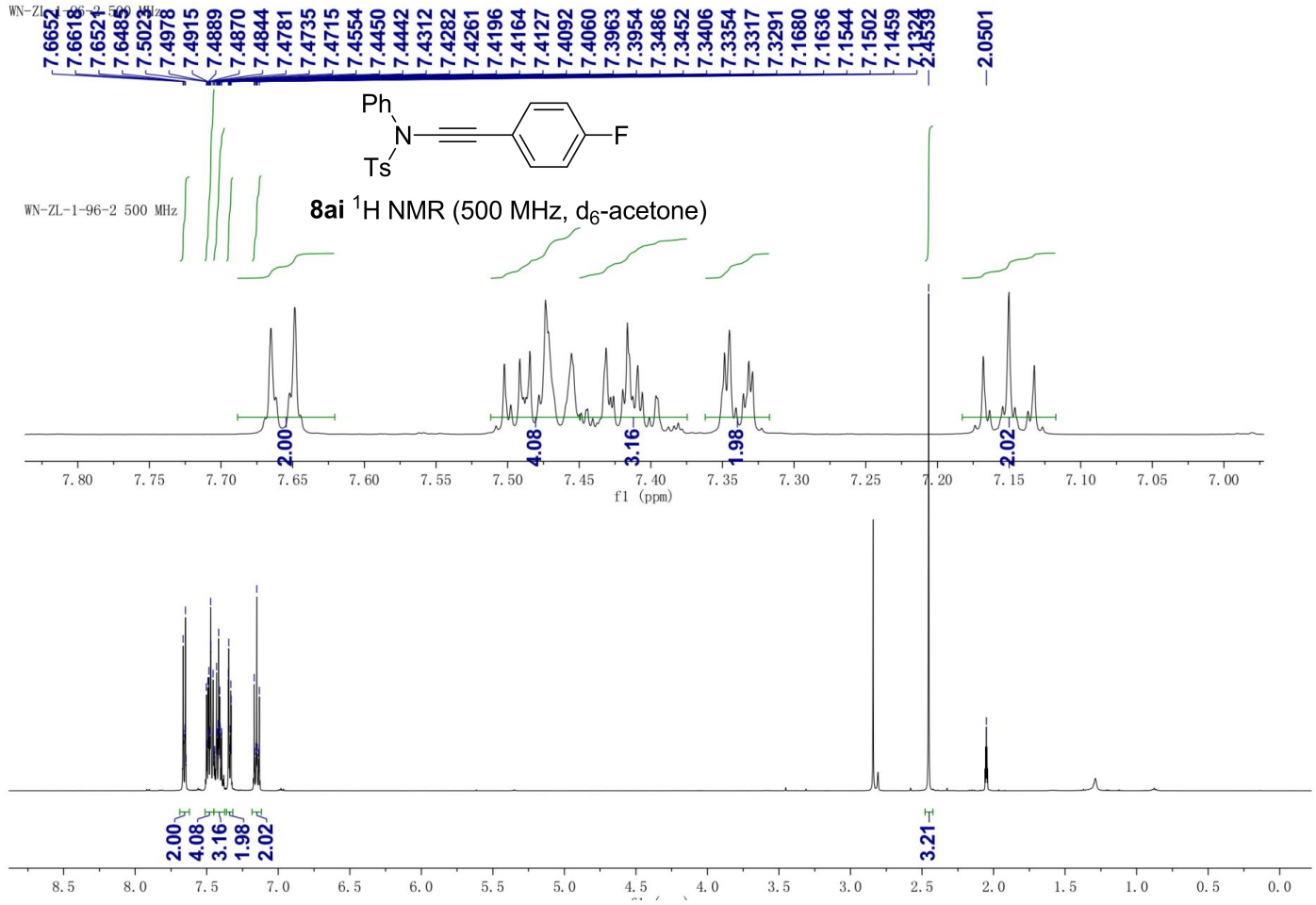
**8ag** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)

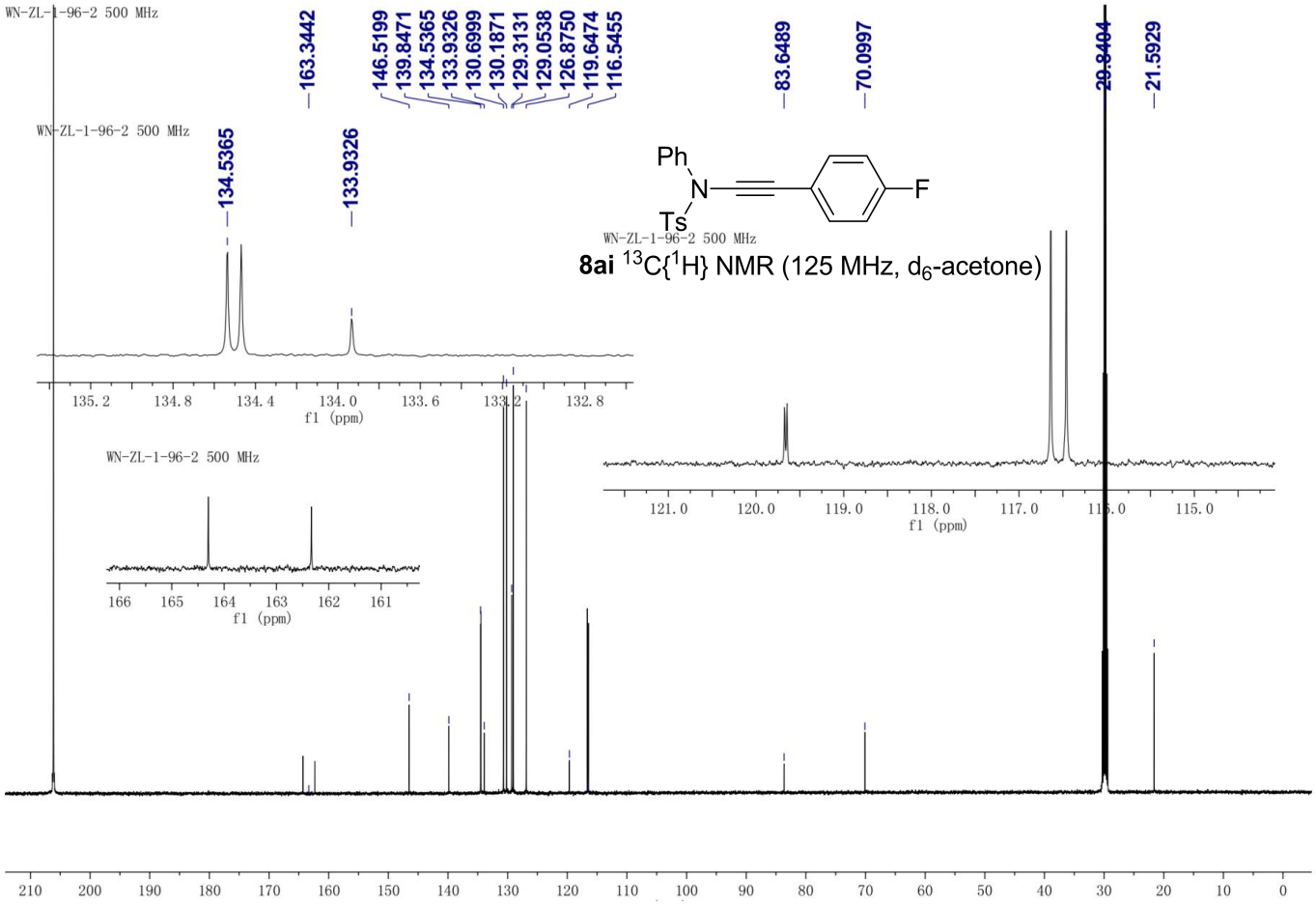


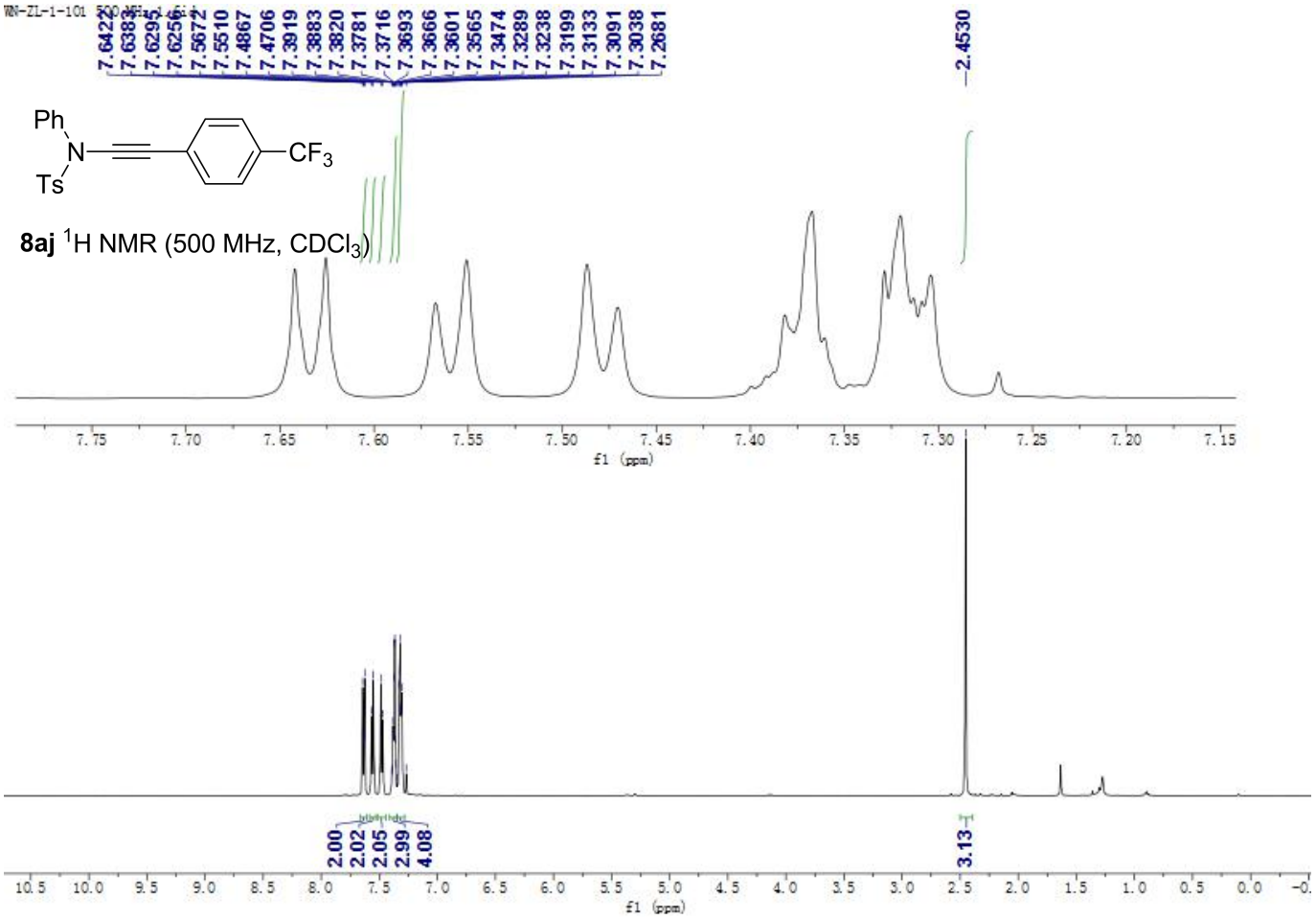

**8ah** $^{1}$H NMR (500 MHz, $CDCl_3$)



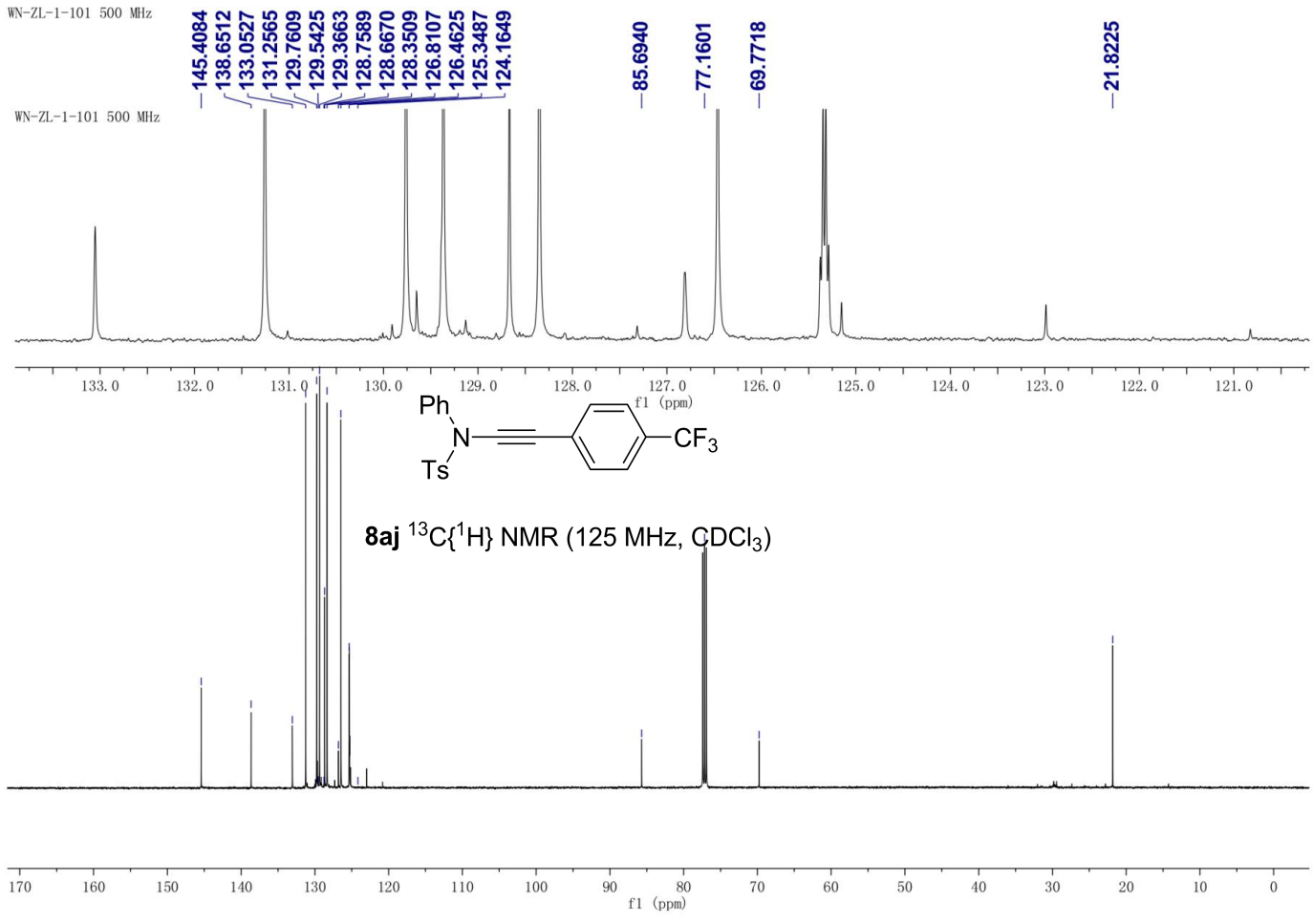

**8ah** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)


Ph
N
Ts
F
WN-ZL-1-96-2 500 MHz
8ai $^{1}$H NMR (500 MHz, $d_6$-acetone)
2.00
4.08
3.16
1.98
2.02
3.21

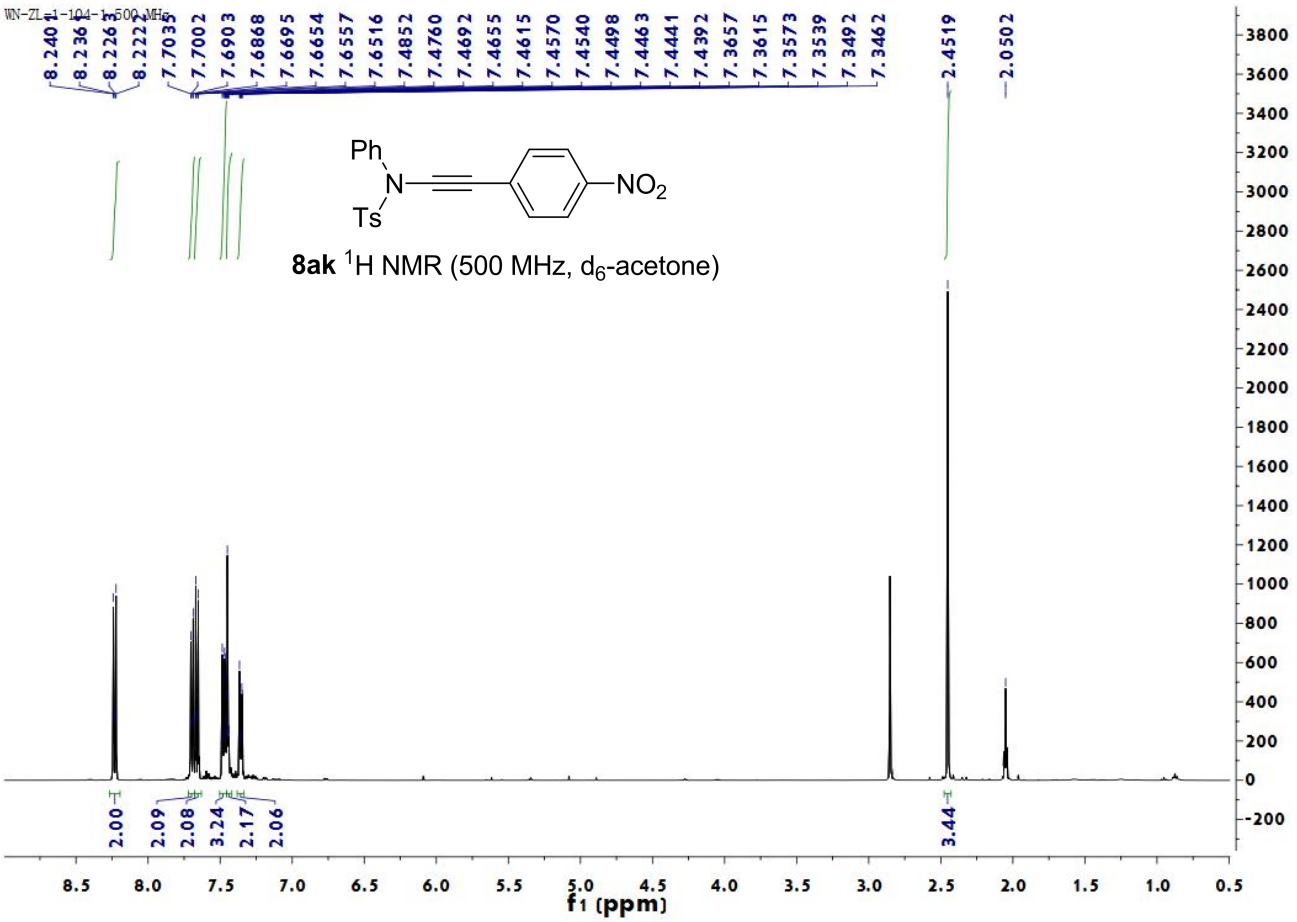

WN-ZL-1-96-2 500 MHz
Ph
N
Ts
F
8ai $^{13}$C{$^{1}$H} NMR (125 MHz, $d_6$-acetone)
f1 (ppm)



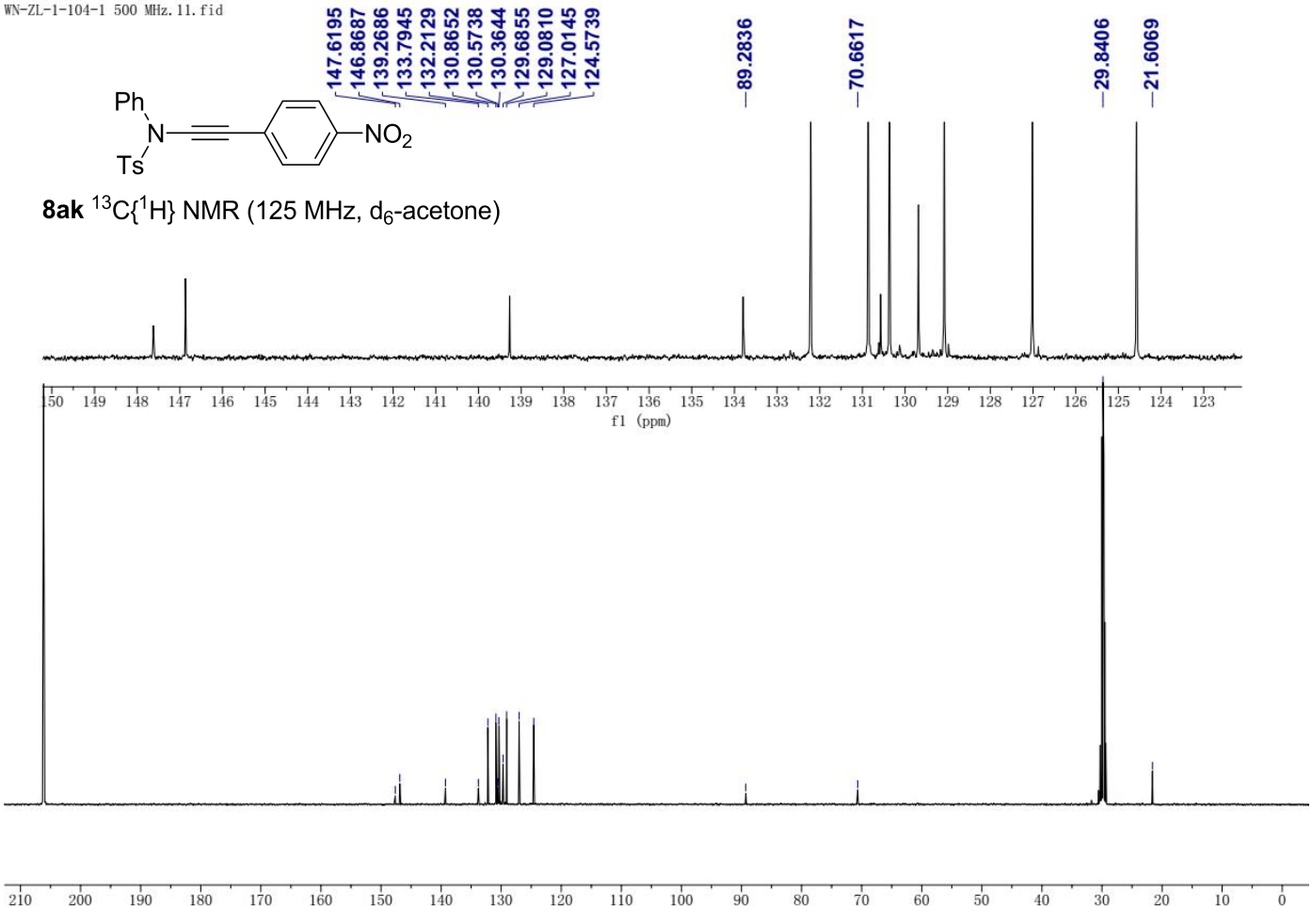

**8aj** $^{1}$H NMR (500 MHz, $CDCl_3$)



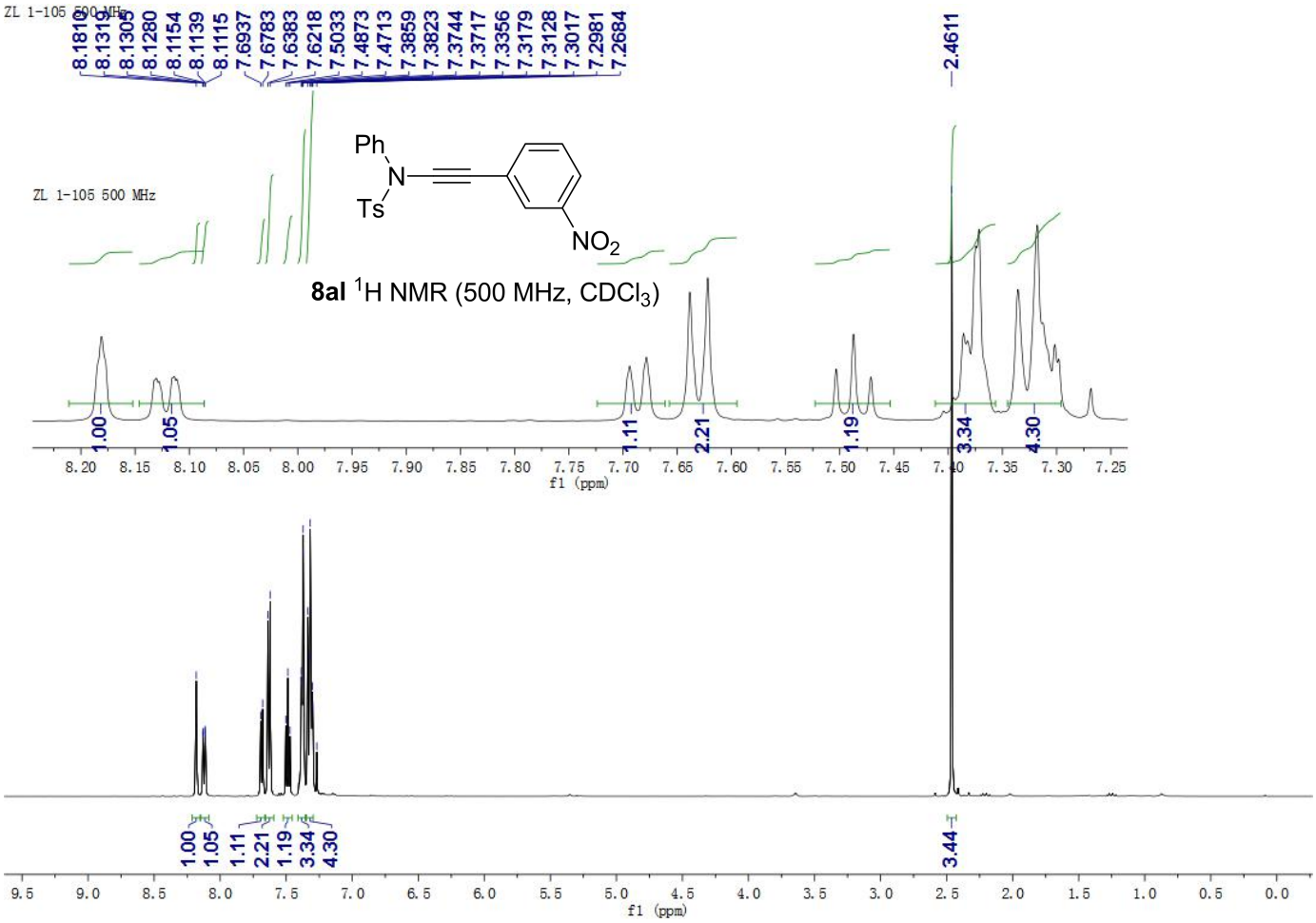

**8aj** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



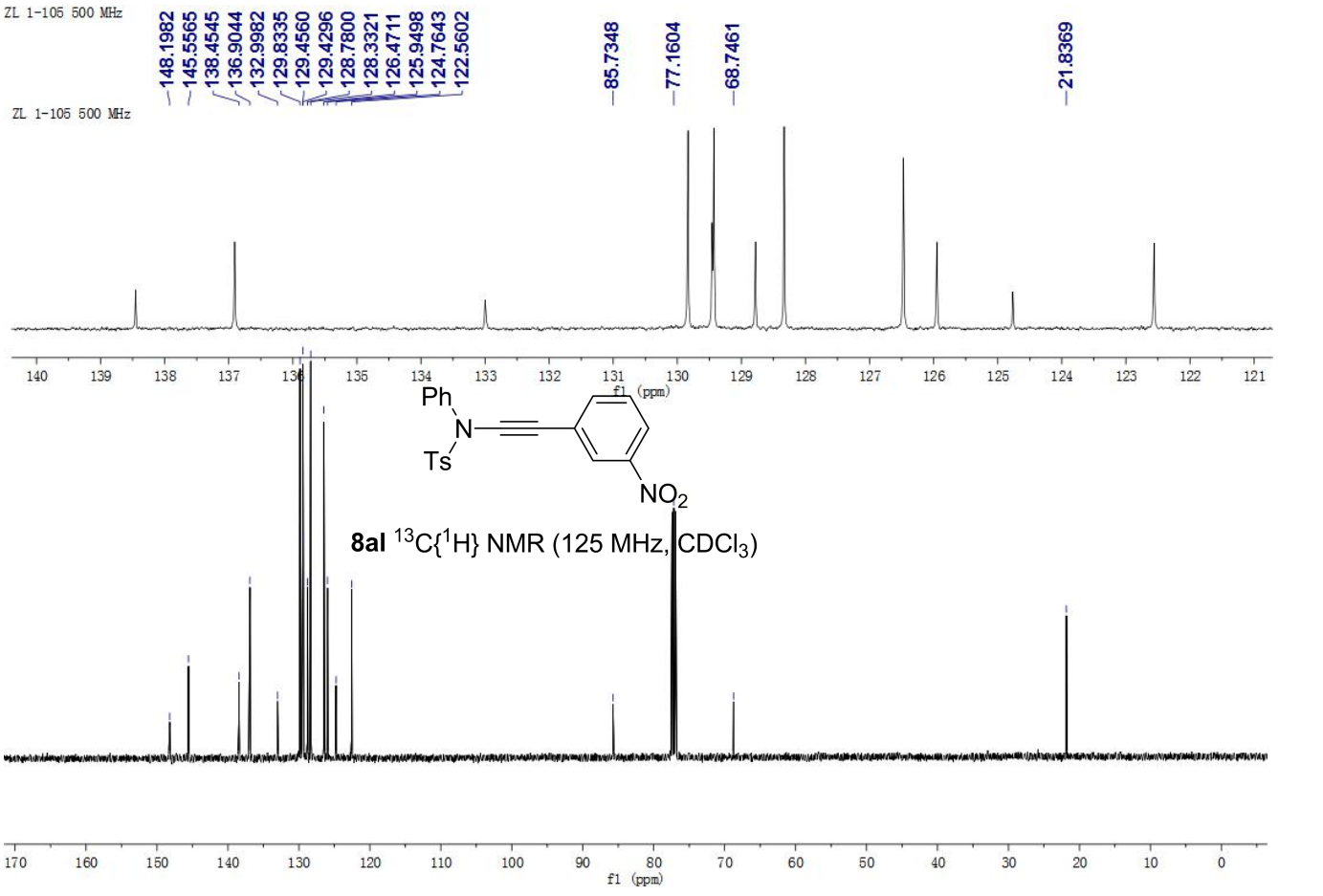

**8ak** $^{1}$H NMR (500 MHz, $d_6$-acetone)



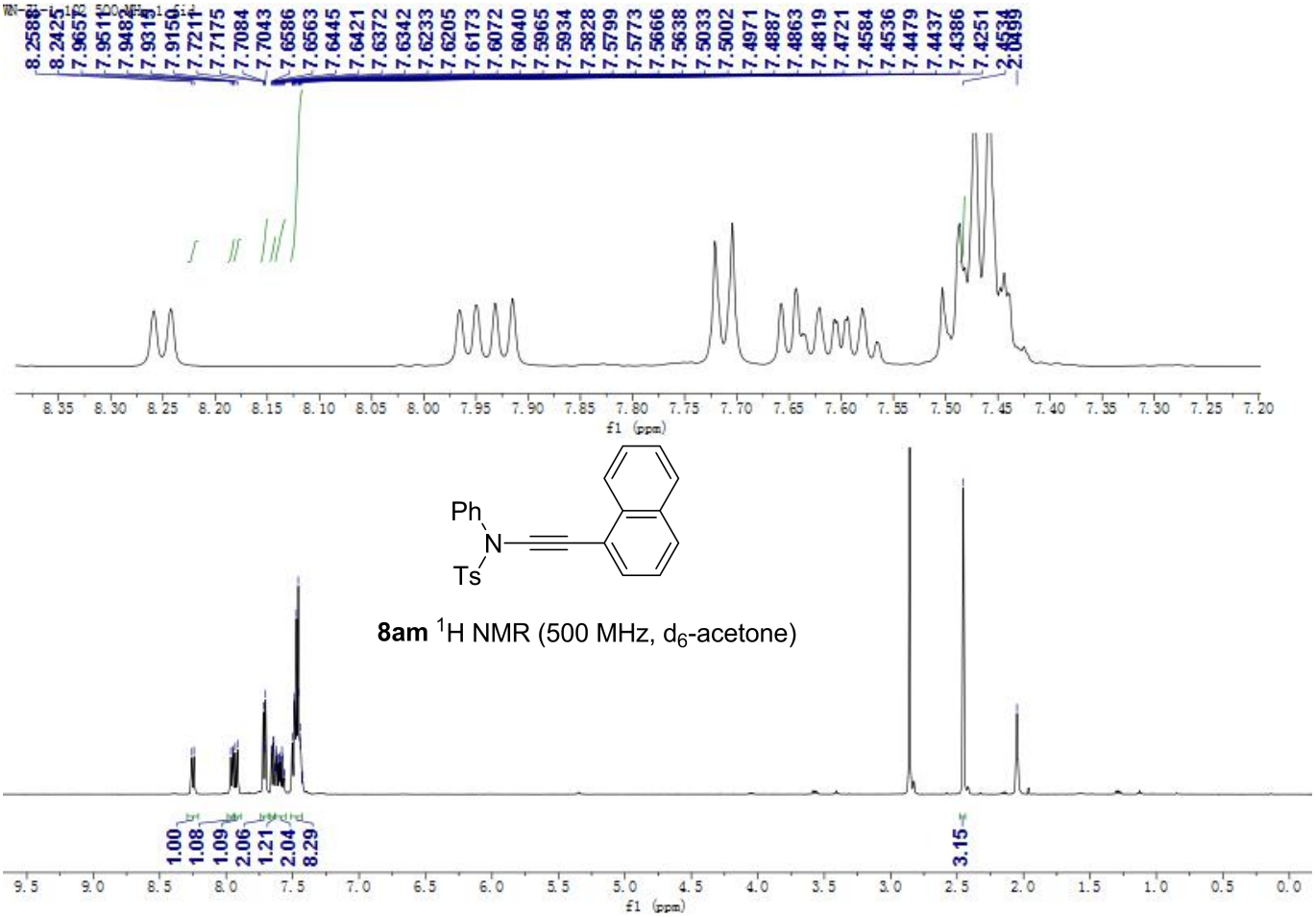

**8ak** $^{13}$C{$^{1}$H} NMR (125 MHz, $d_6$-acetone)



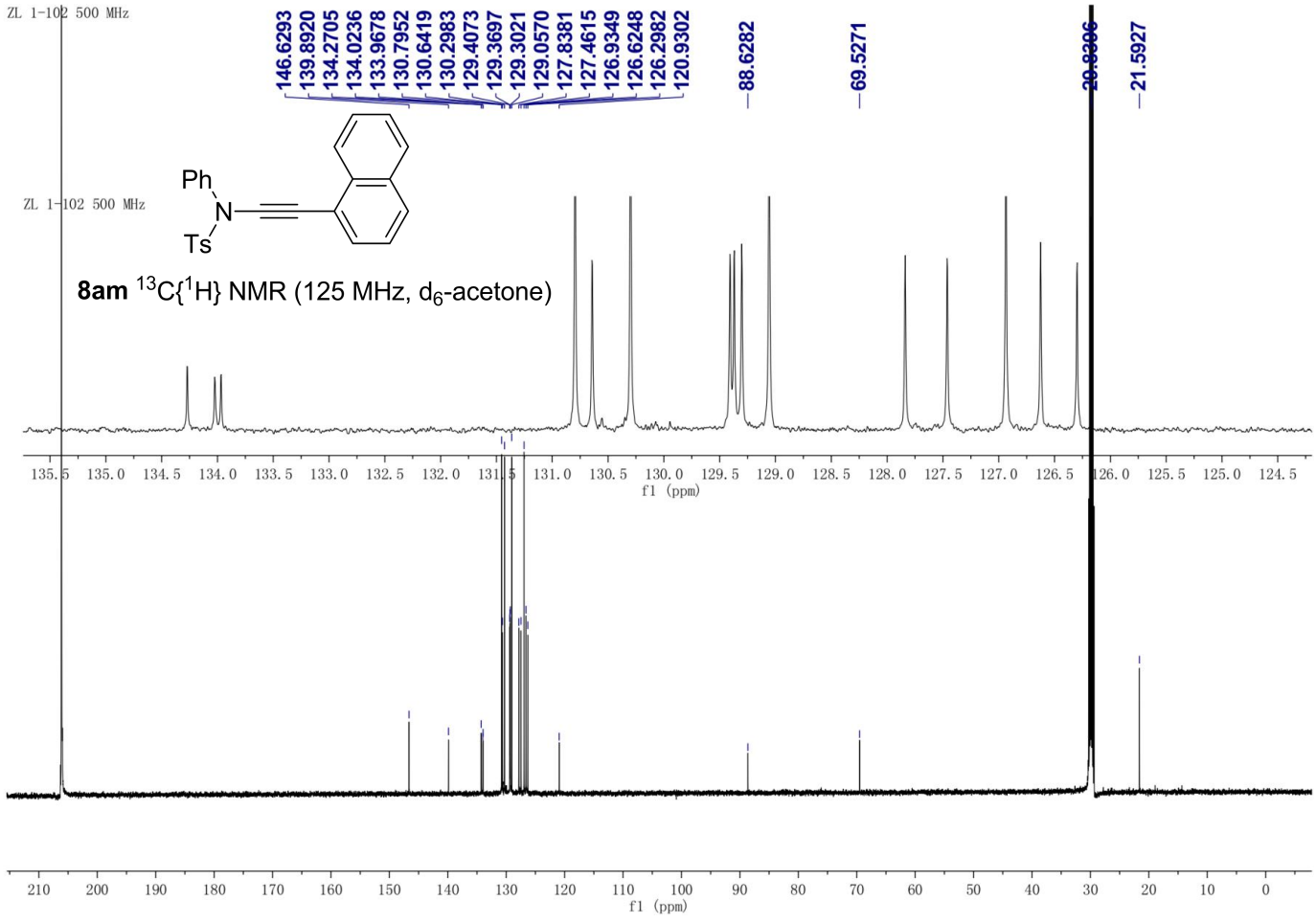

**8al** $^{1}$H NMR (500 MHz, $CDCl_3$)



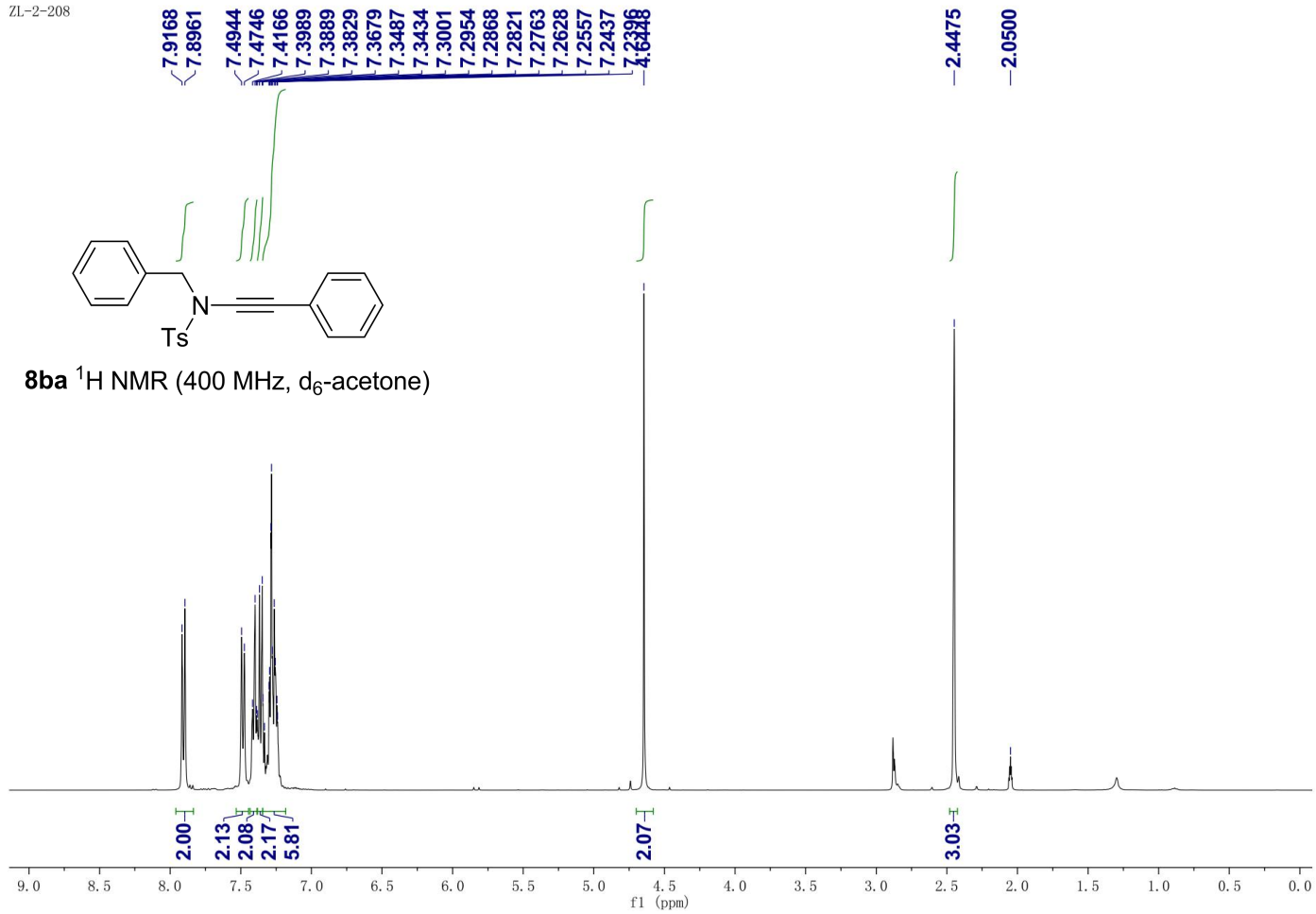

**8al** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



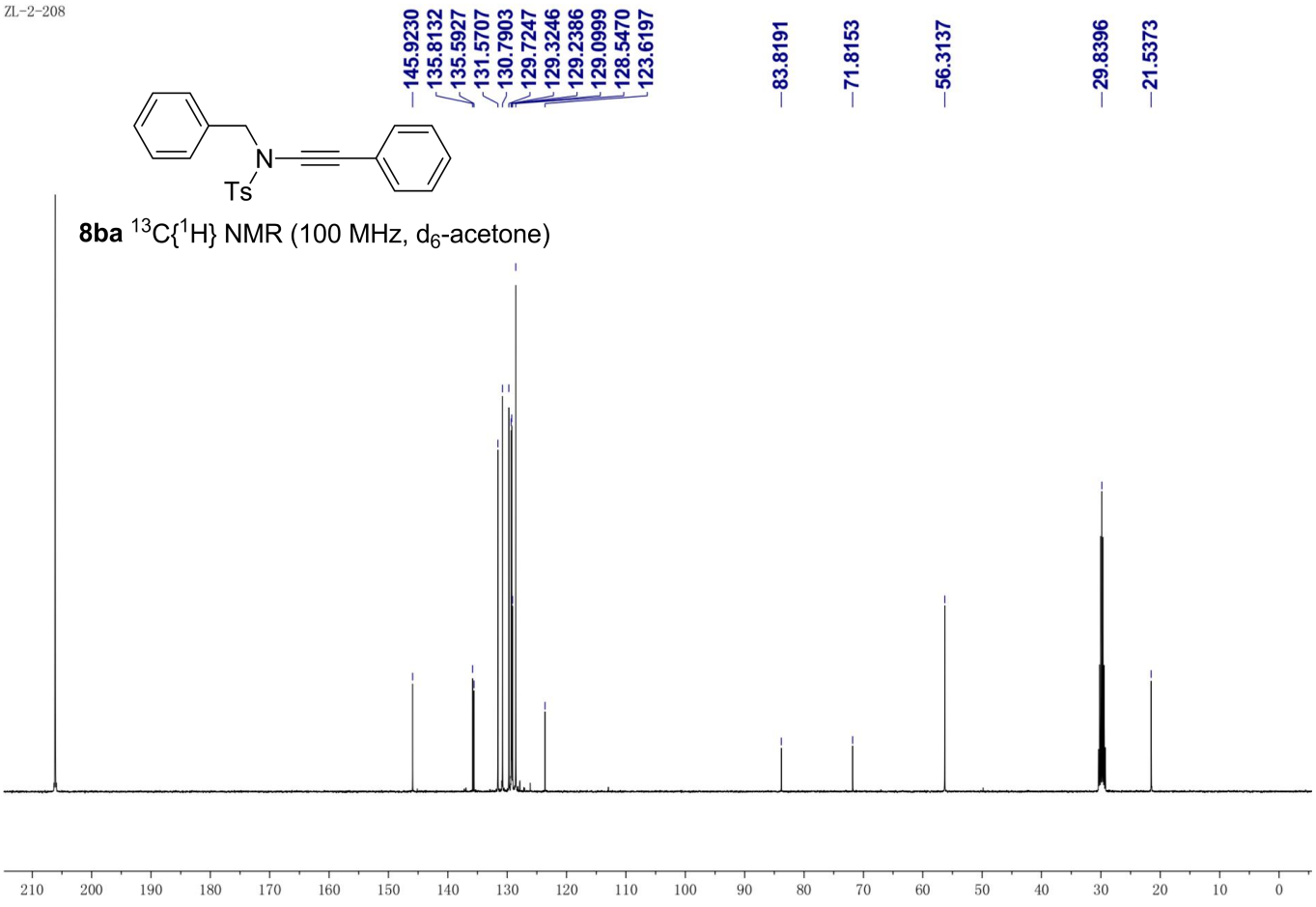

**8am** $^{1}$H NMR (500 MHz, $d_6$-acetone)



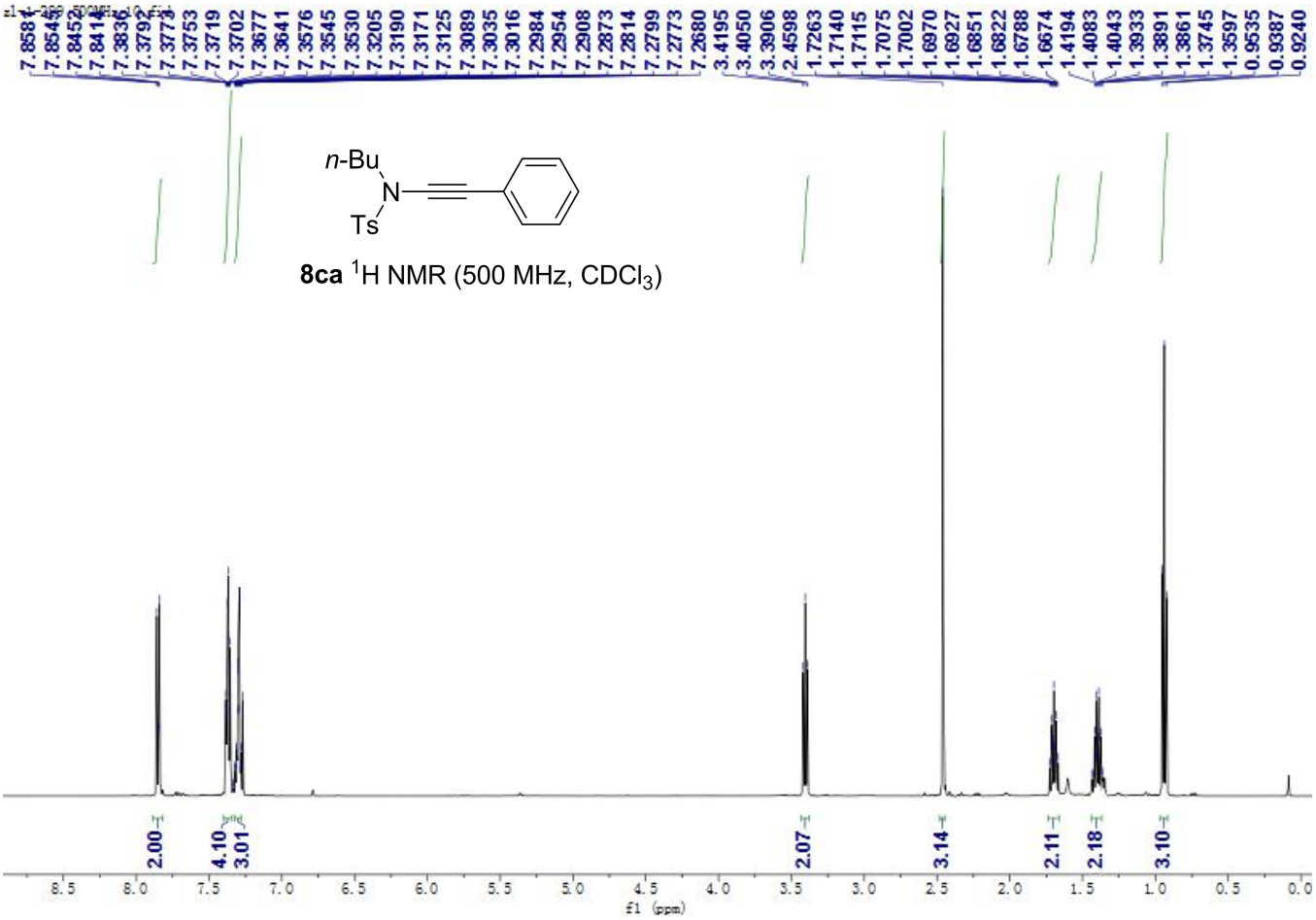

**8am** $^{13}$C{$^{1}$H} NMR (125 MHz, $d_6$-acetone)



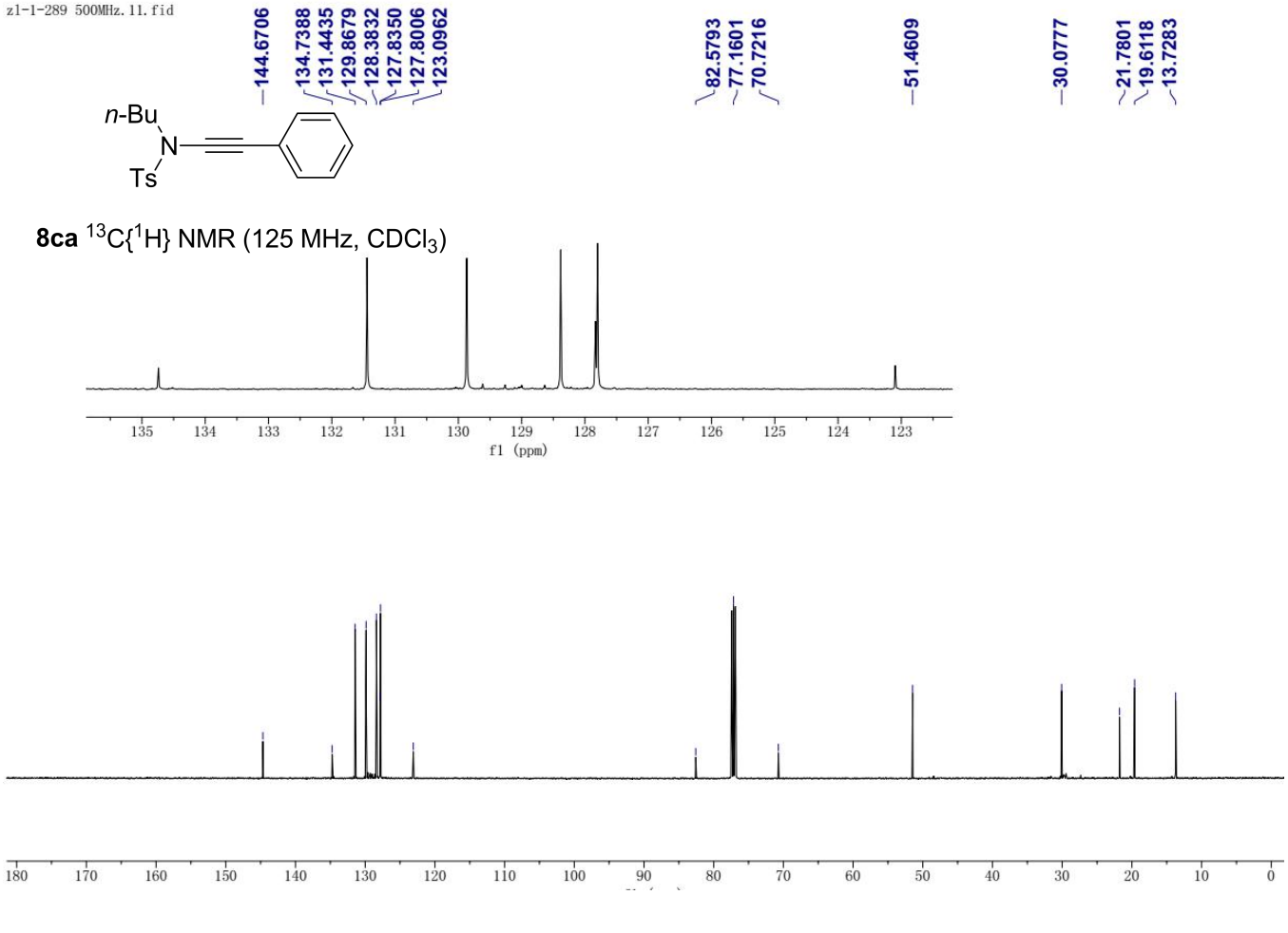

**8ba** $^{1}$H NMR (400 MHz, $d_6$-acetone)



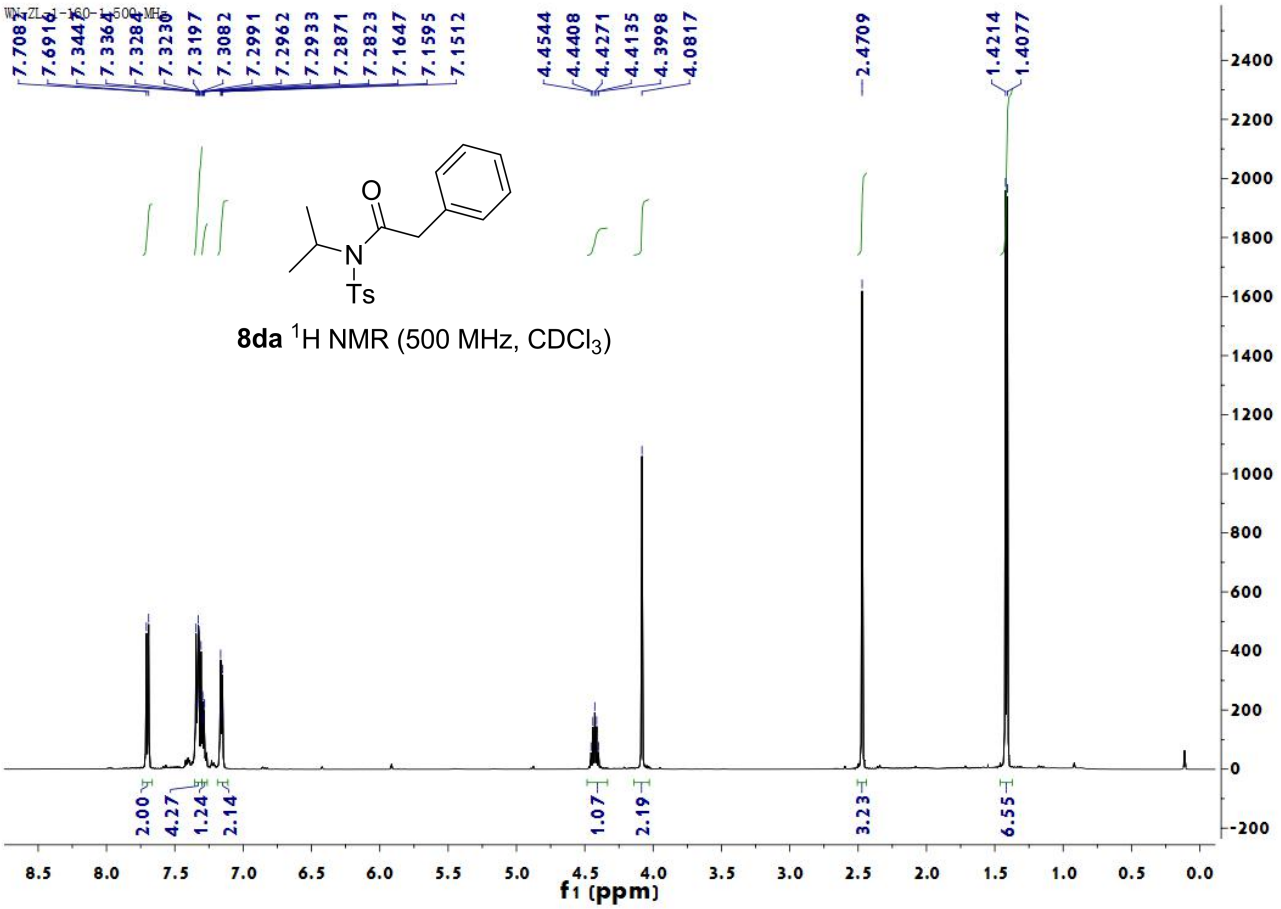

**8ba** $^{13}$C{$^{1}$H} NMR (100 MHz, $d_6$-acetone)



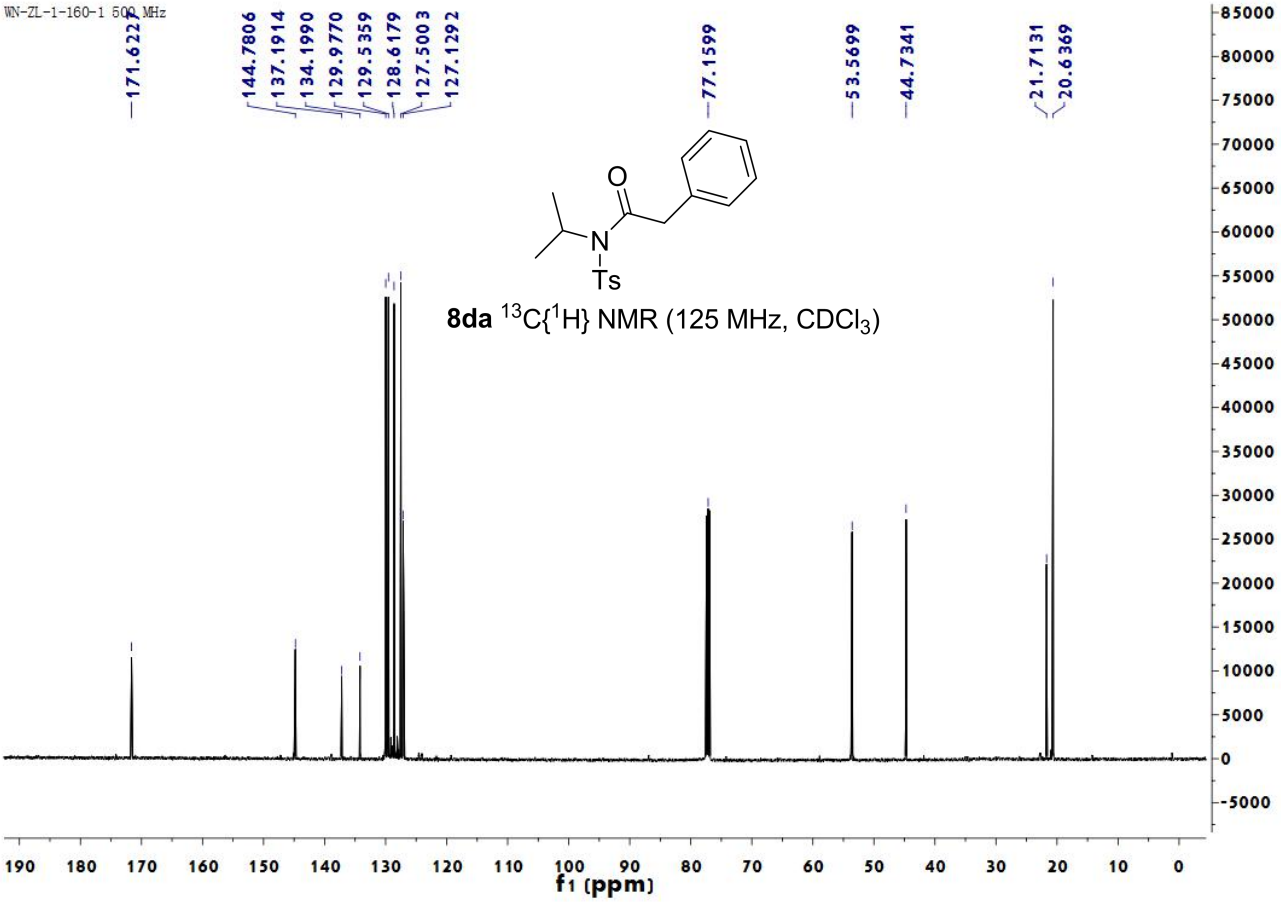

**8ca** $^{1}$H NMR (500 MHz, $CDCl_3$)



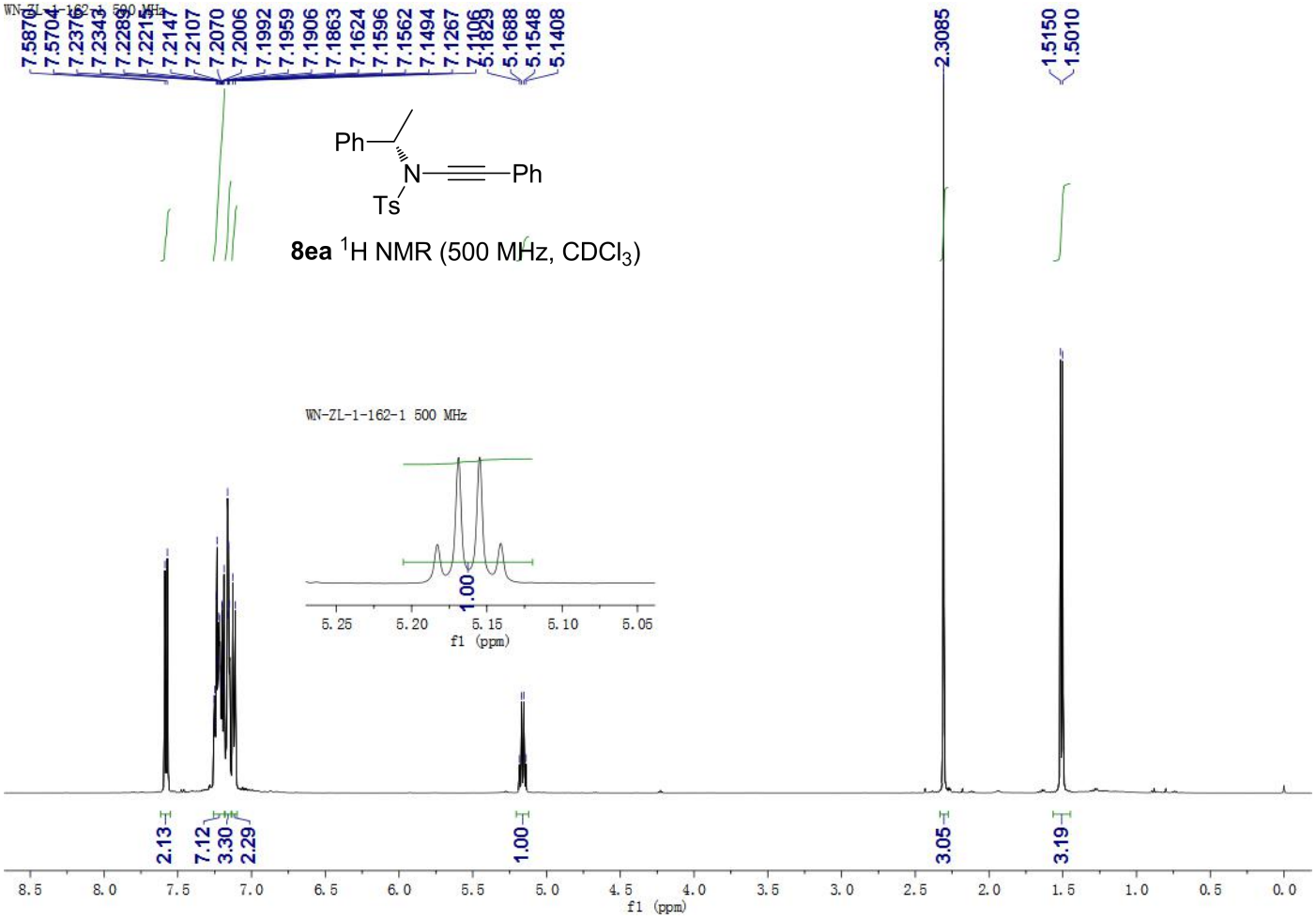

**8ca** $^{13}$C{$^{1}$H} NMR (125 MHz, $CDCl_3$)



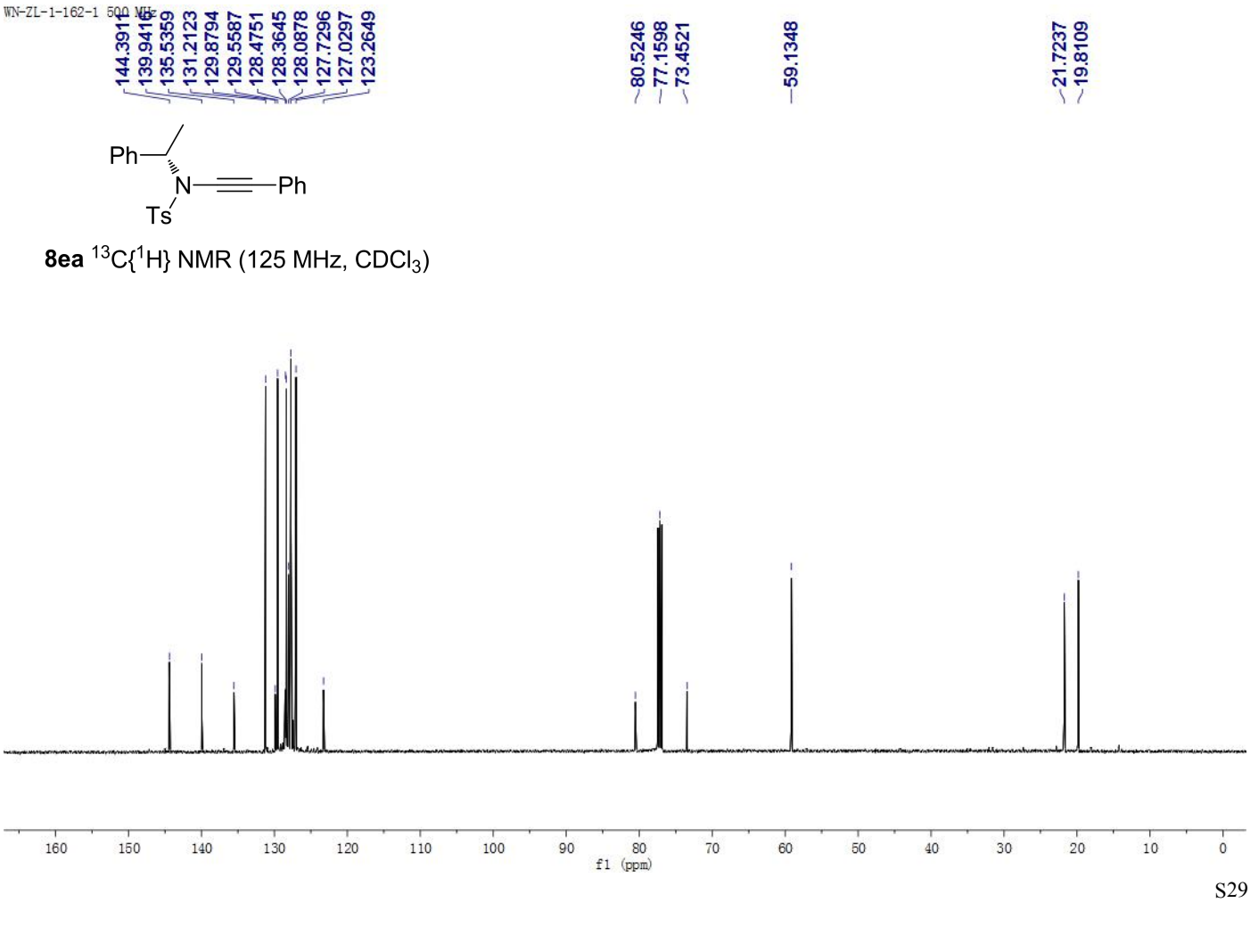

**8da** $^{1}$H NMR (500 MHz, $CDCl_3$)



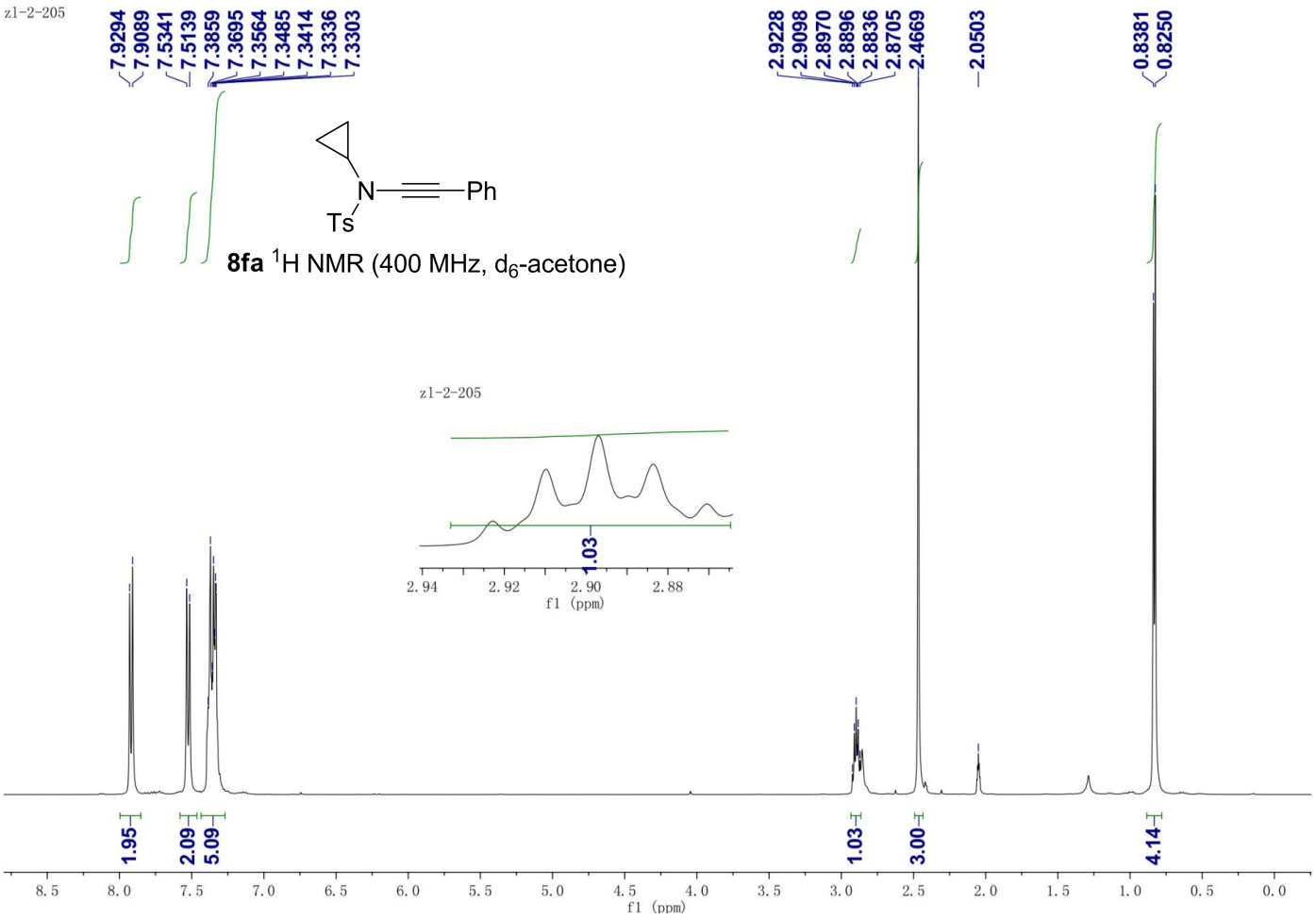

**8da** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



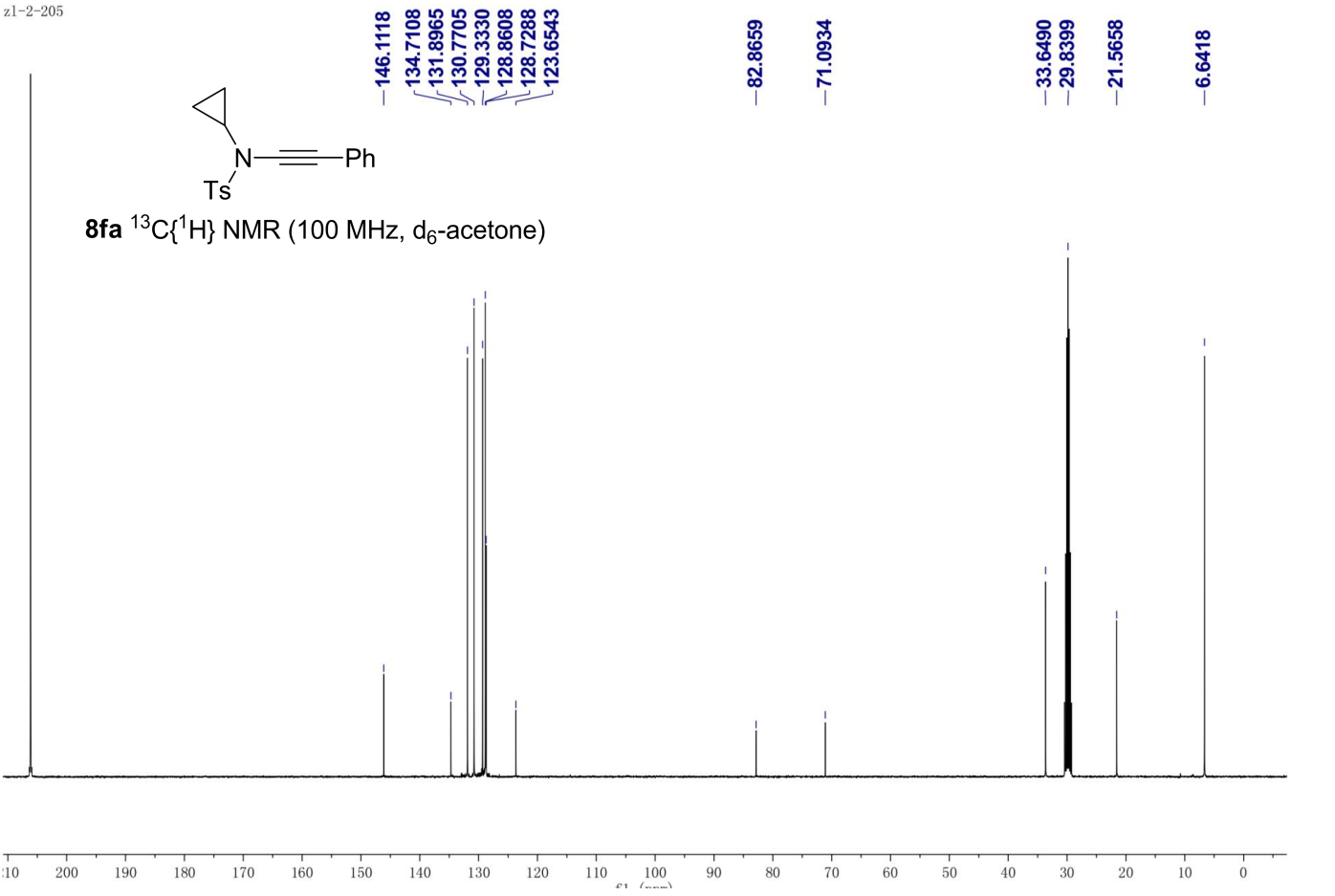

**8ea** $^{1}$H NMR (500 MHz, $CDCl_3$)



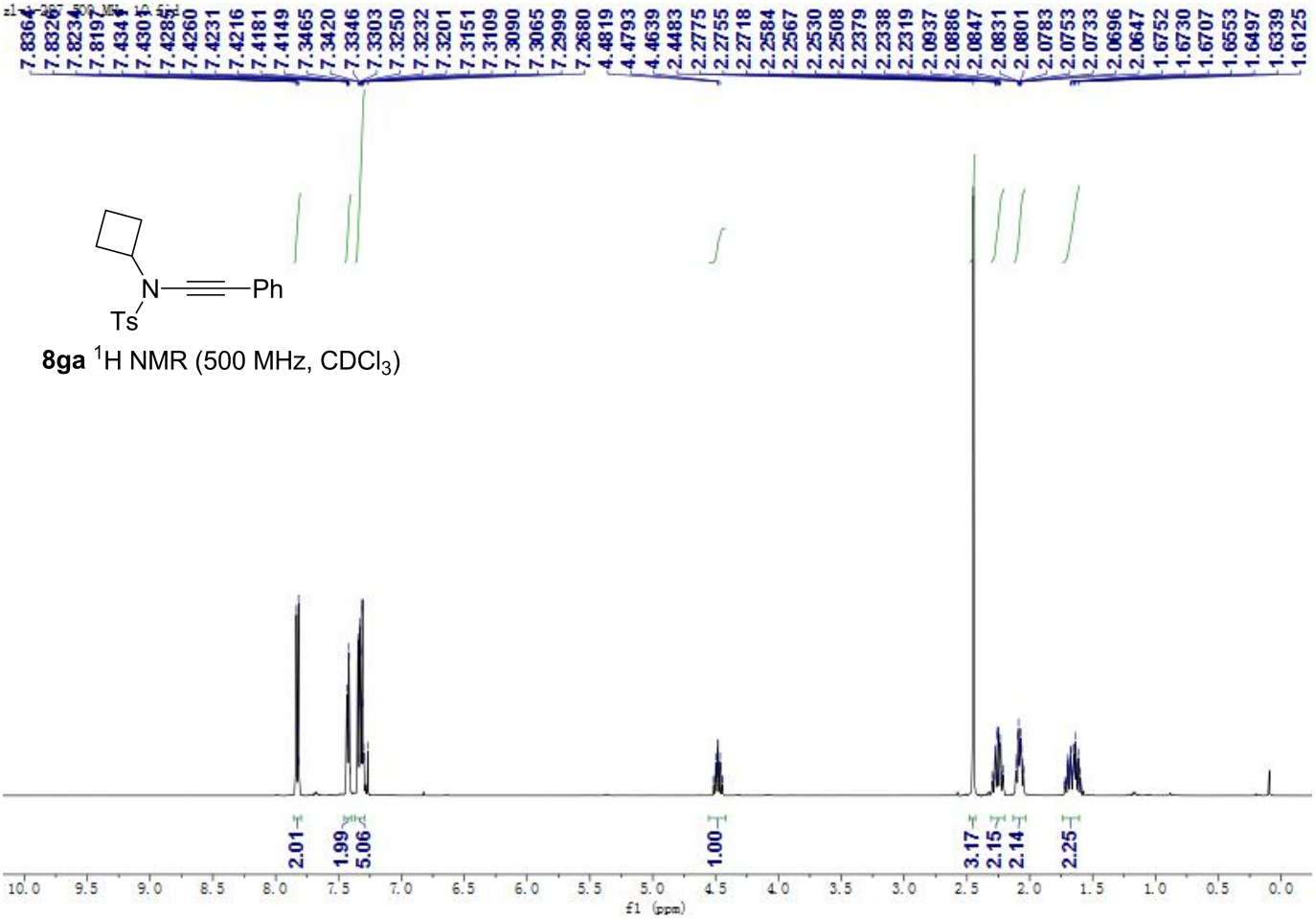

**8ea** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



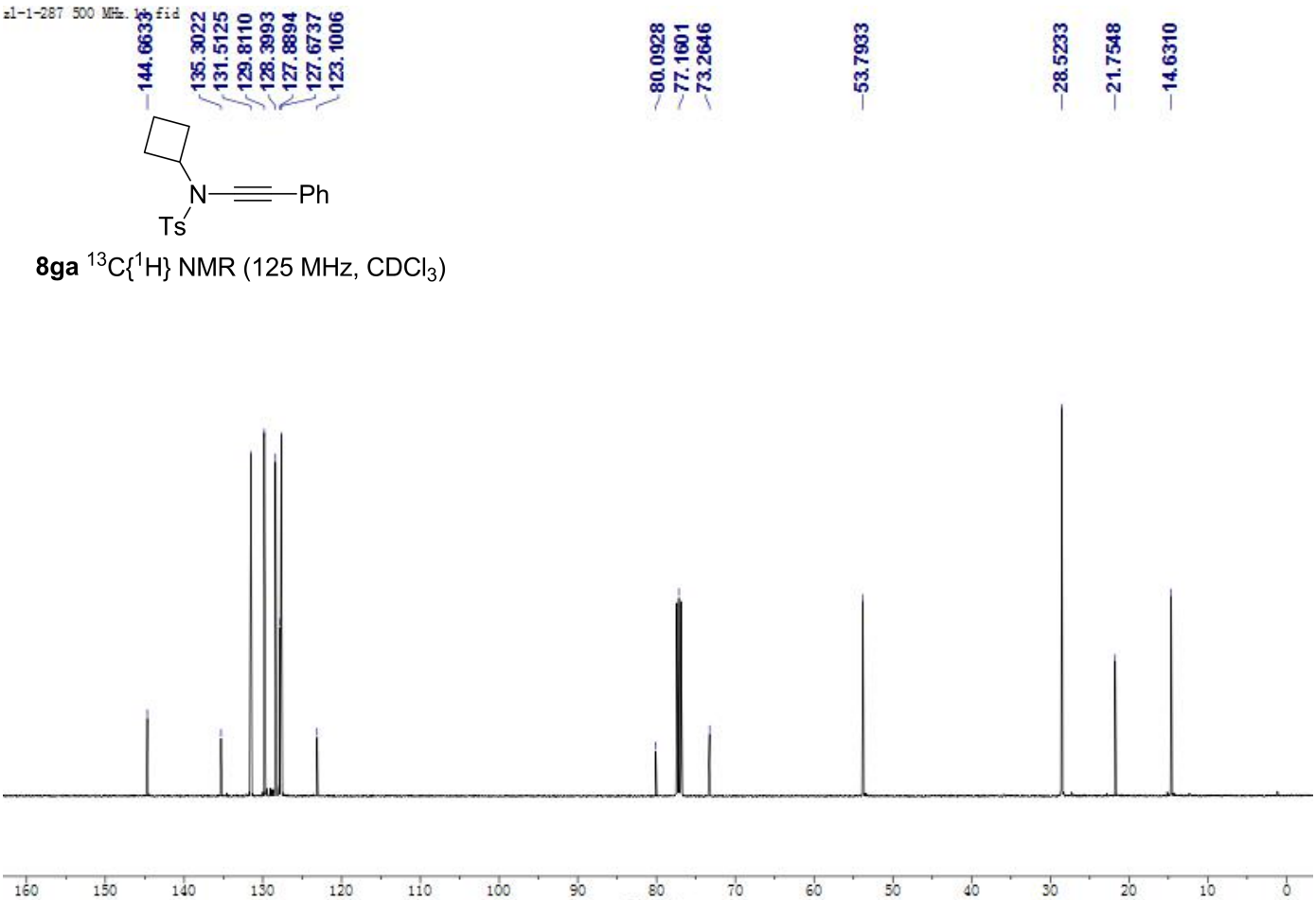

**8fa** $^{1}$H NMR (400 MHz, $d_6$-acetone)



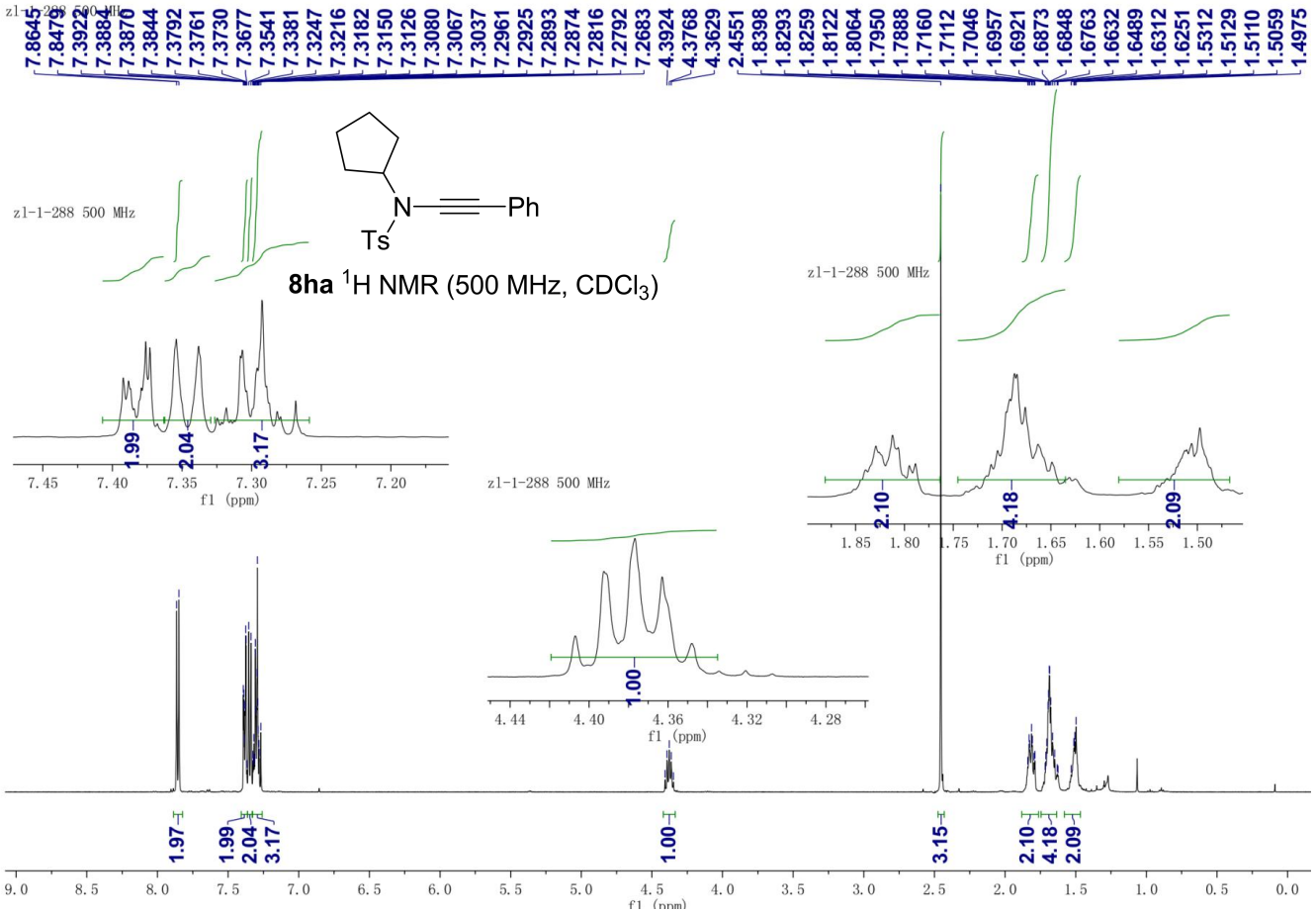

**8fa** $^{13}$C{$^{1}$H} NMR (100 MHz, $d_6$-acetone)



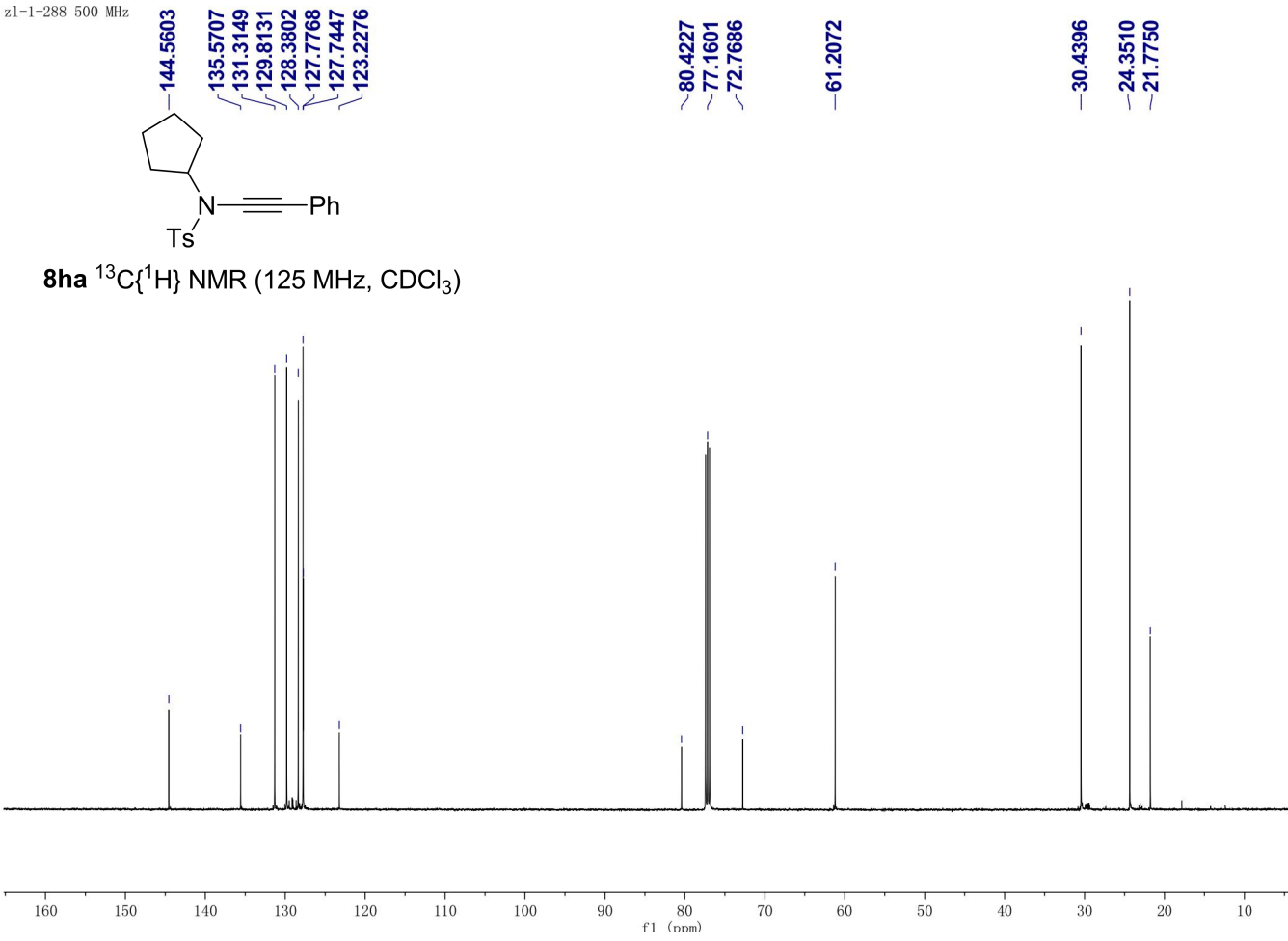

**8ga** $^{1}$H NMR (500 MHz, $CDCl_3$)



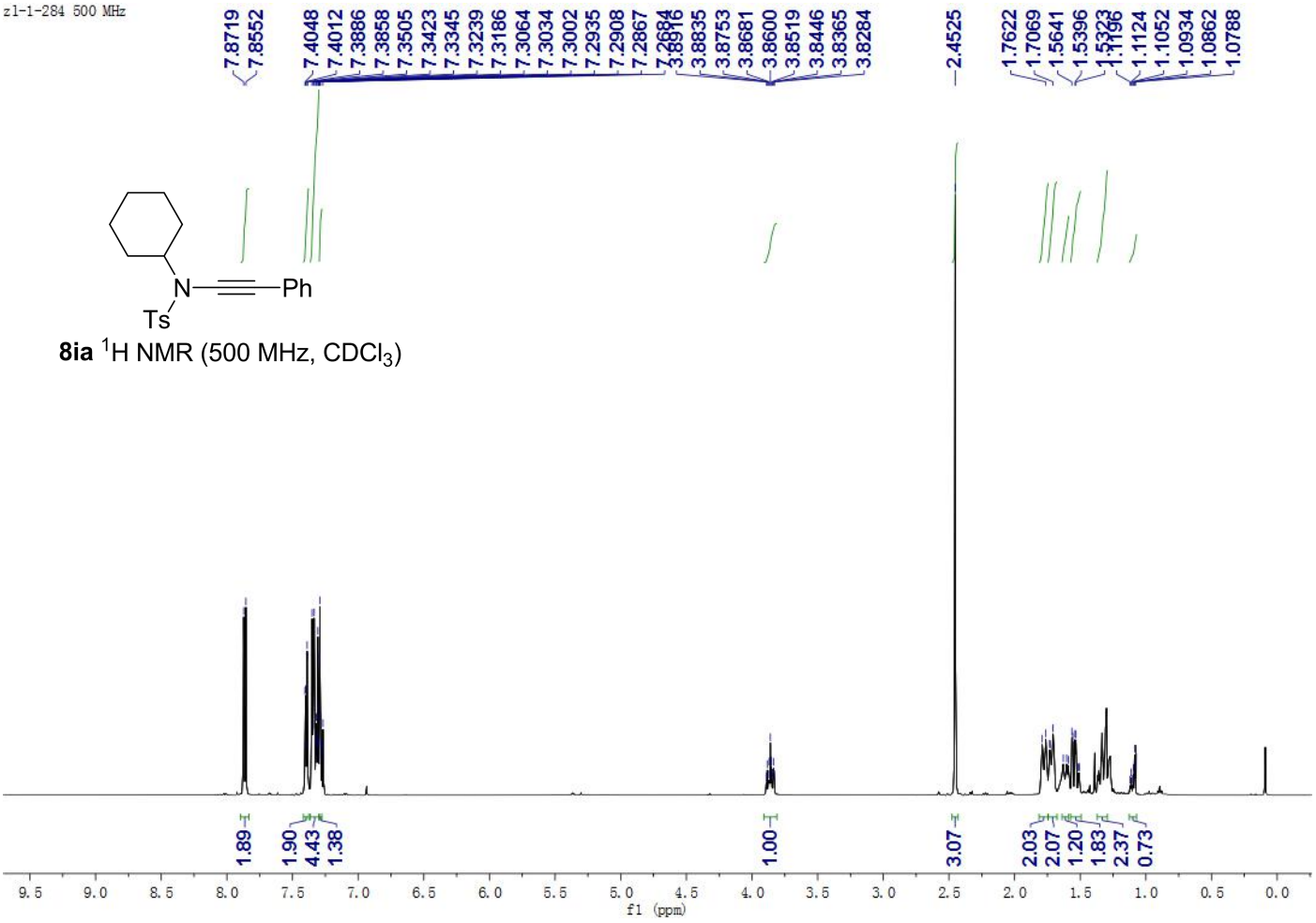

**8ga** $^{13}$C{$^{1}$H} NMR (125 MHz, $CDCl_3$)



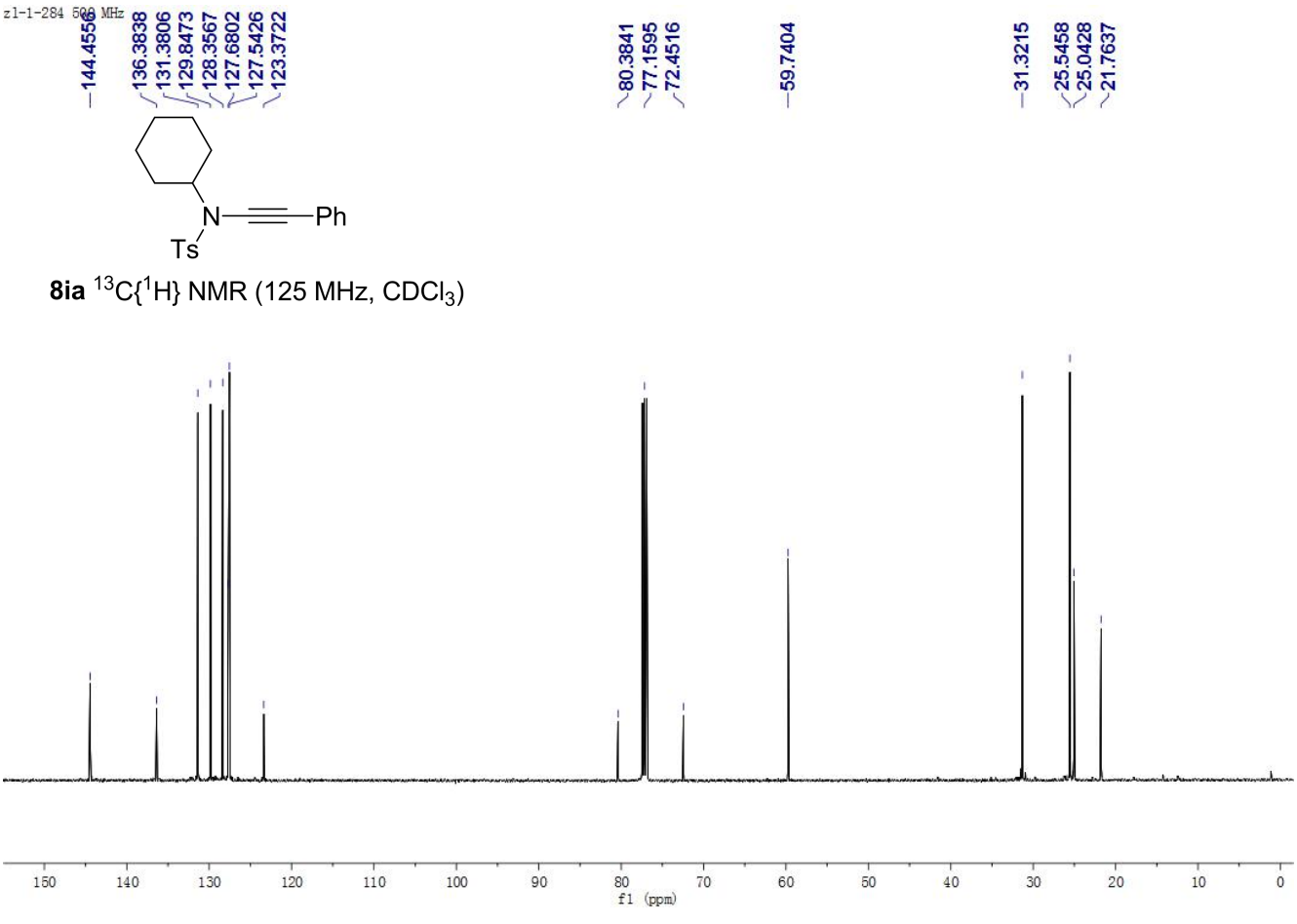

**8ha** $^{1}$H NMR (500 MHz, $CDCl_3$)



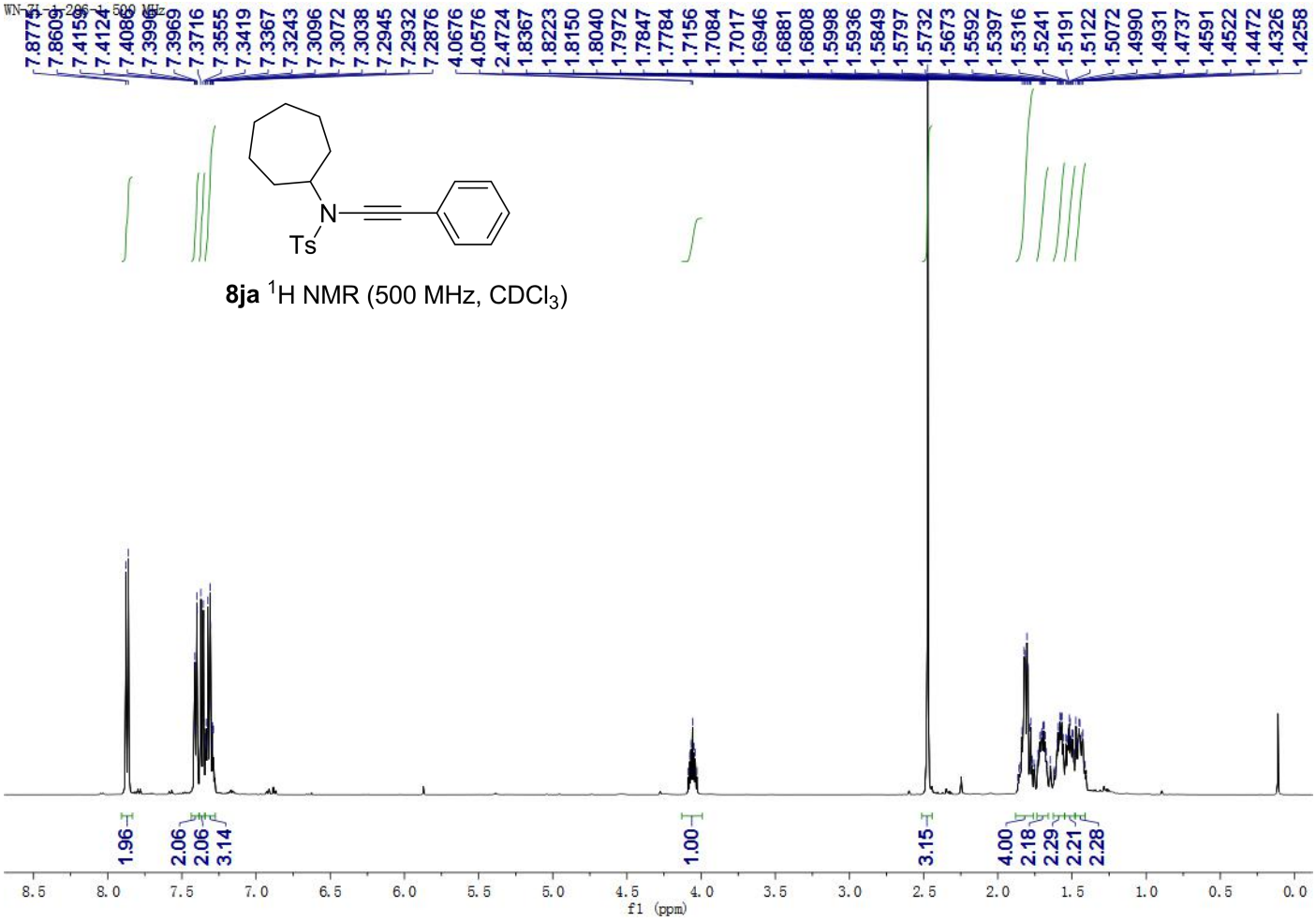

**8ha** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



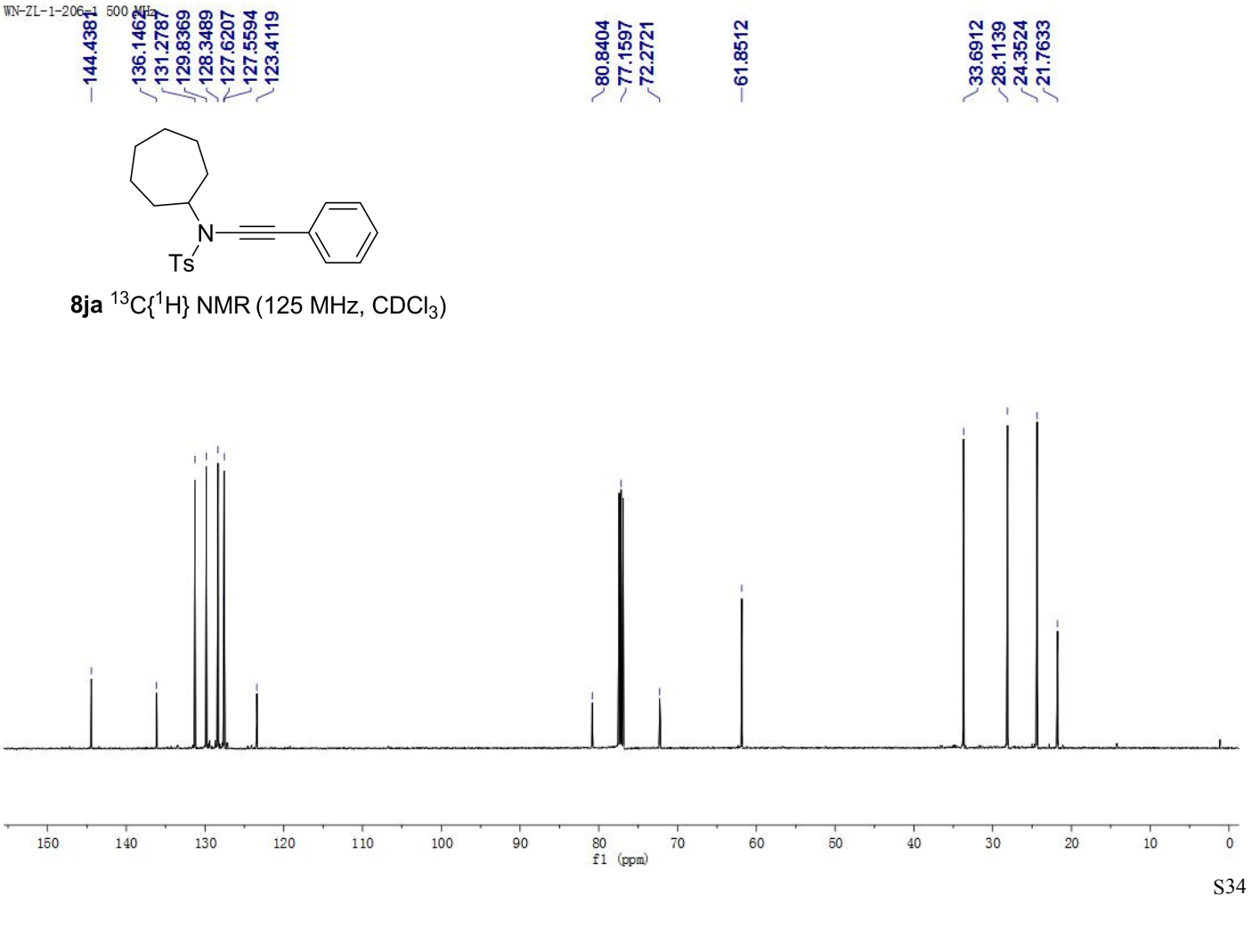

**8ia** $^{1}$H NMR (500 MHz, $CDCl_3$)



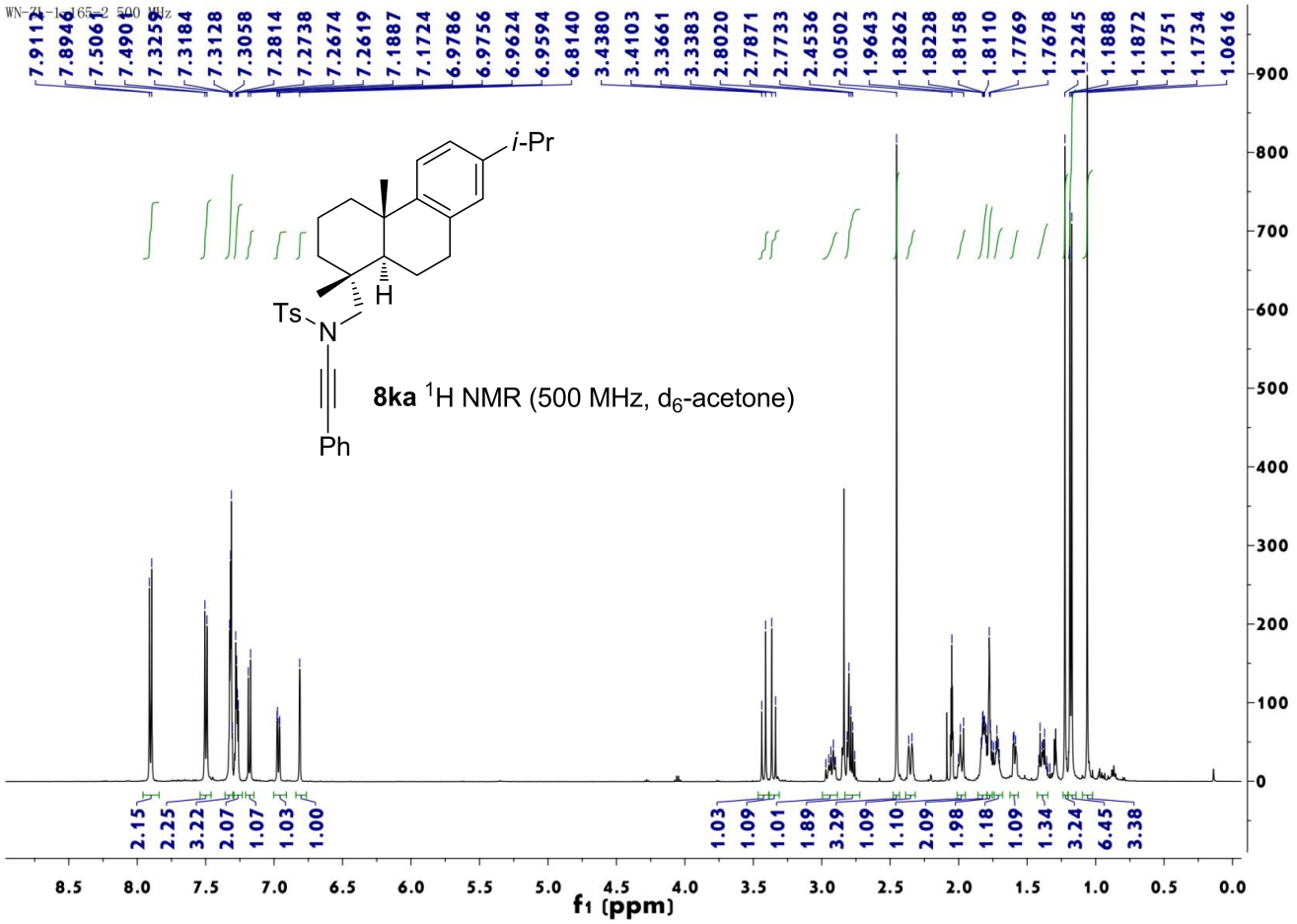

**8ia** $^{13}$C{$^{1}$H} NMR (125 MHz, $CDCl_3$)

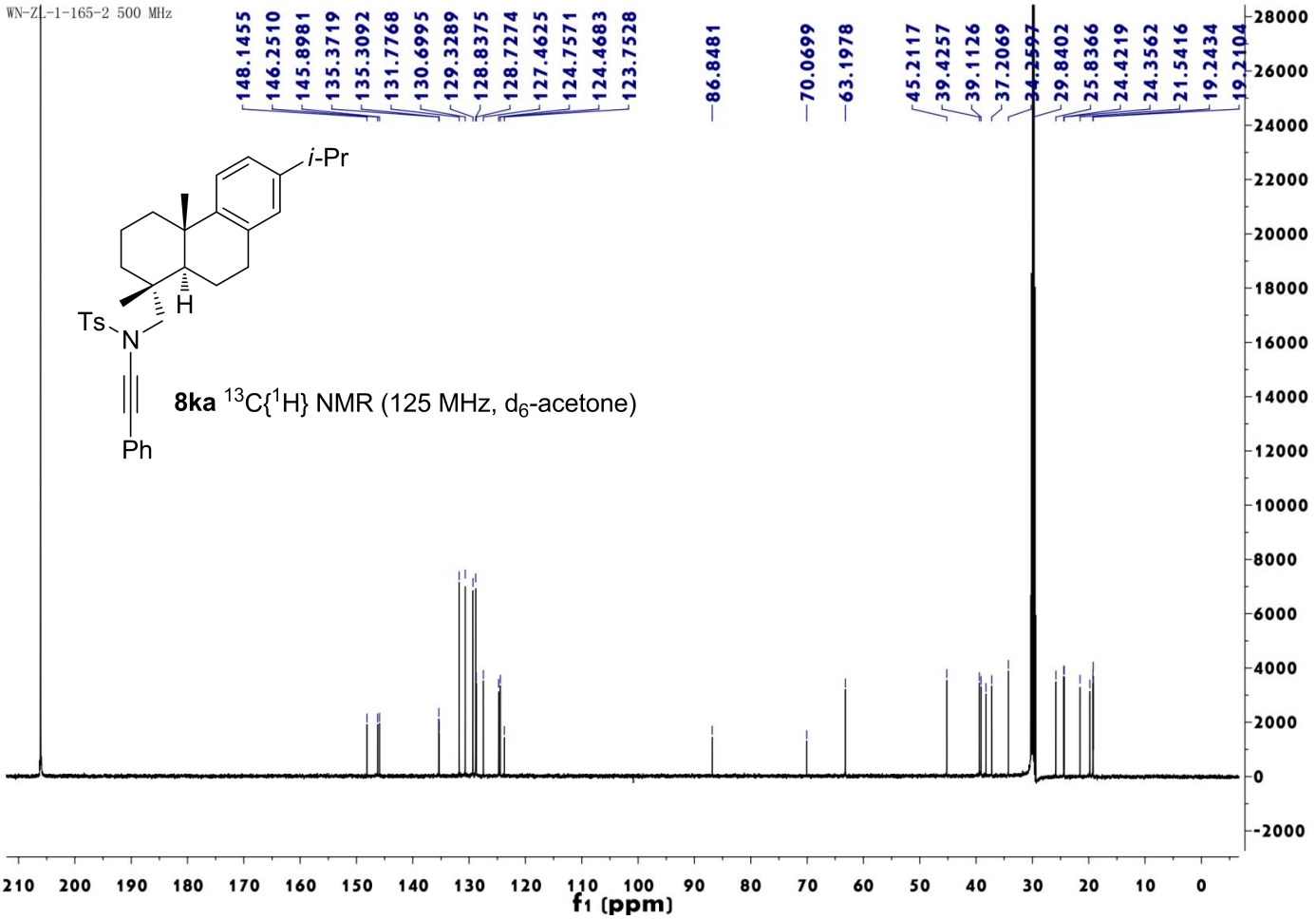


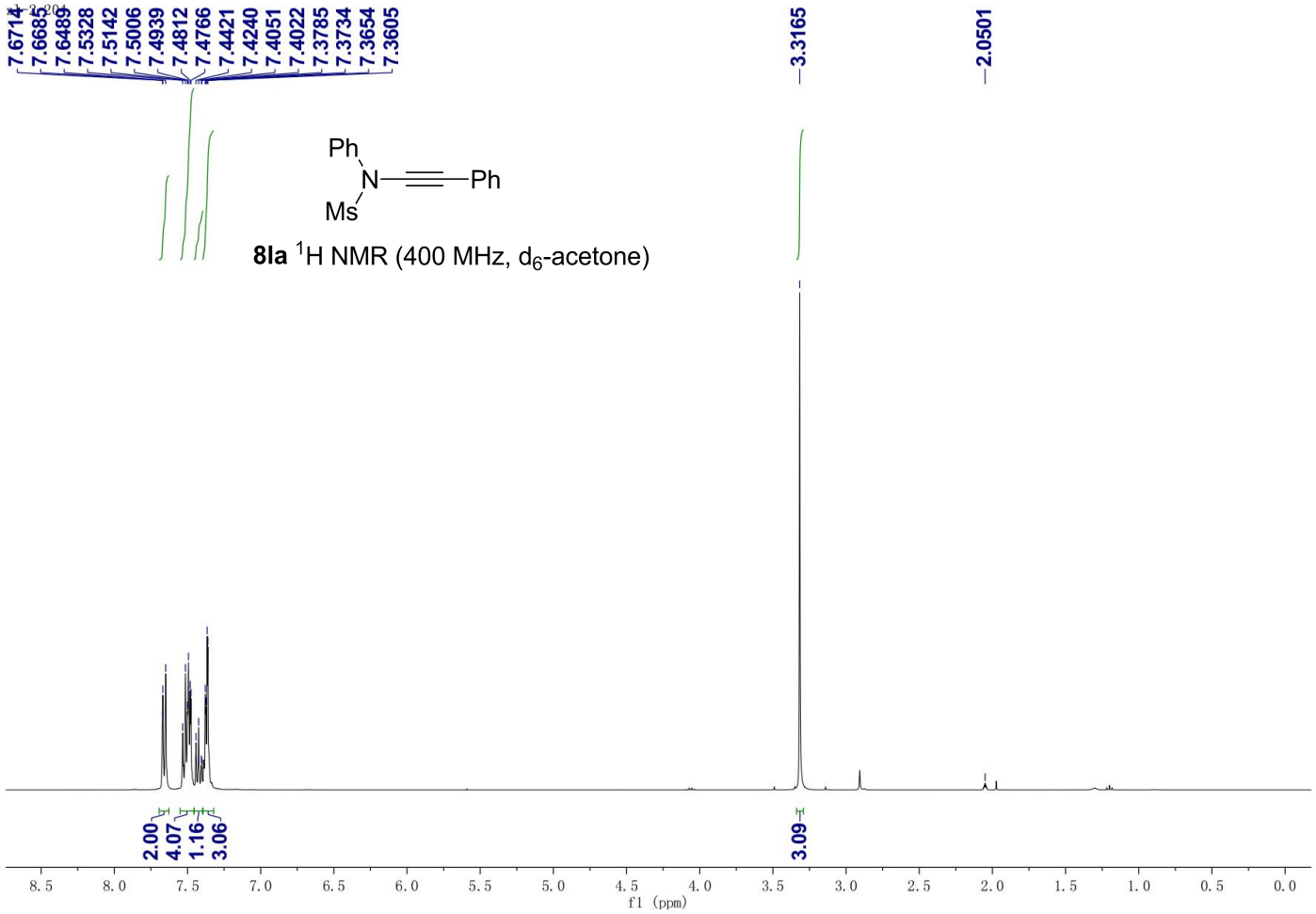

**8ja** $^{1}$H NMR (500 MHz, $CDCl_3$)



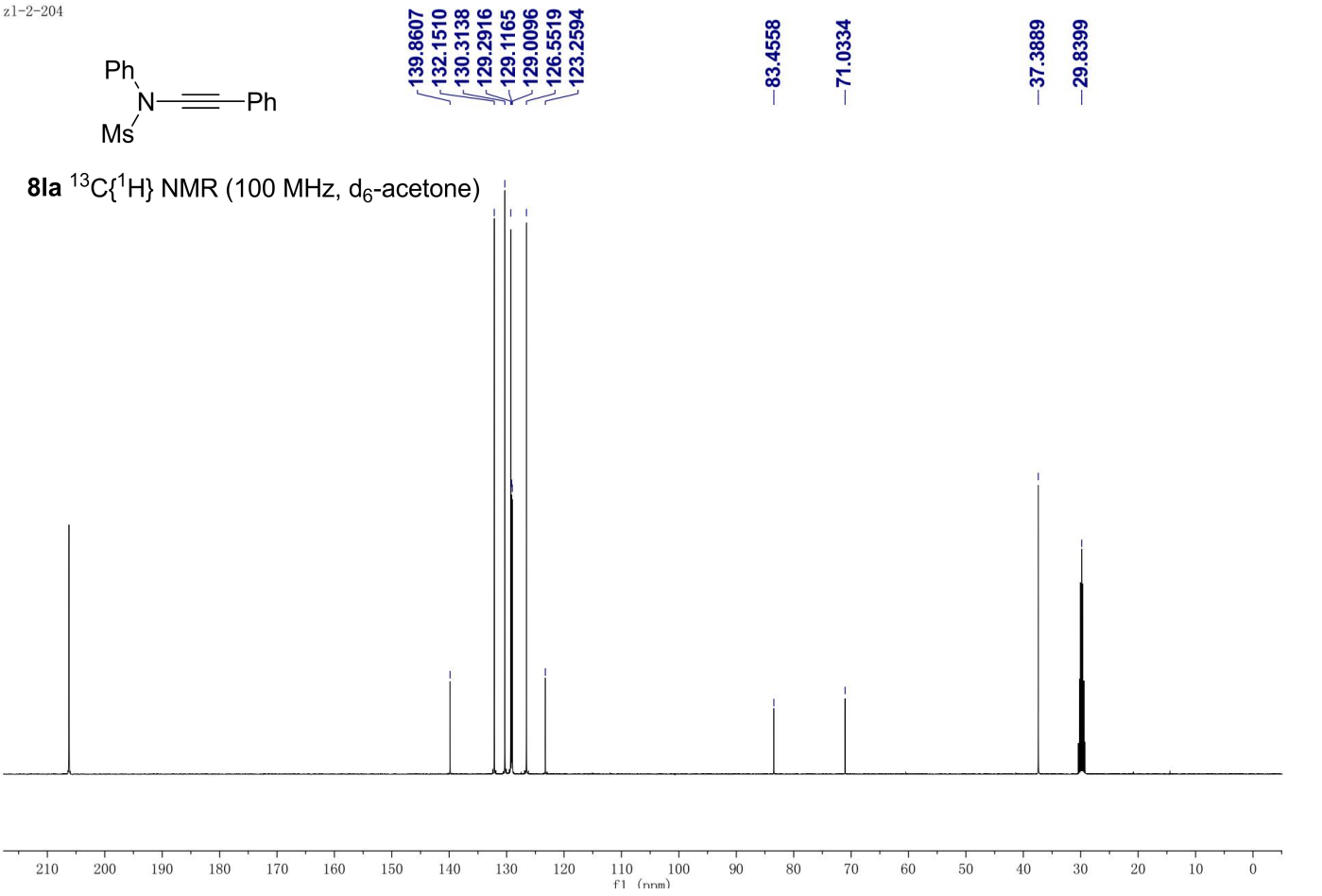

**8ja** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)


i-Pr
Ts
N
H
Ph
8ka $^{1}$H NMR (500 MHz, $d_6$-acetone)
f1 (ppm)

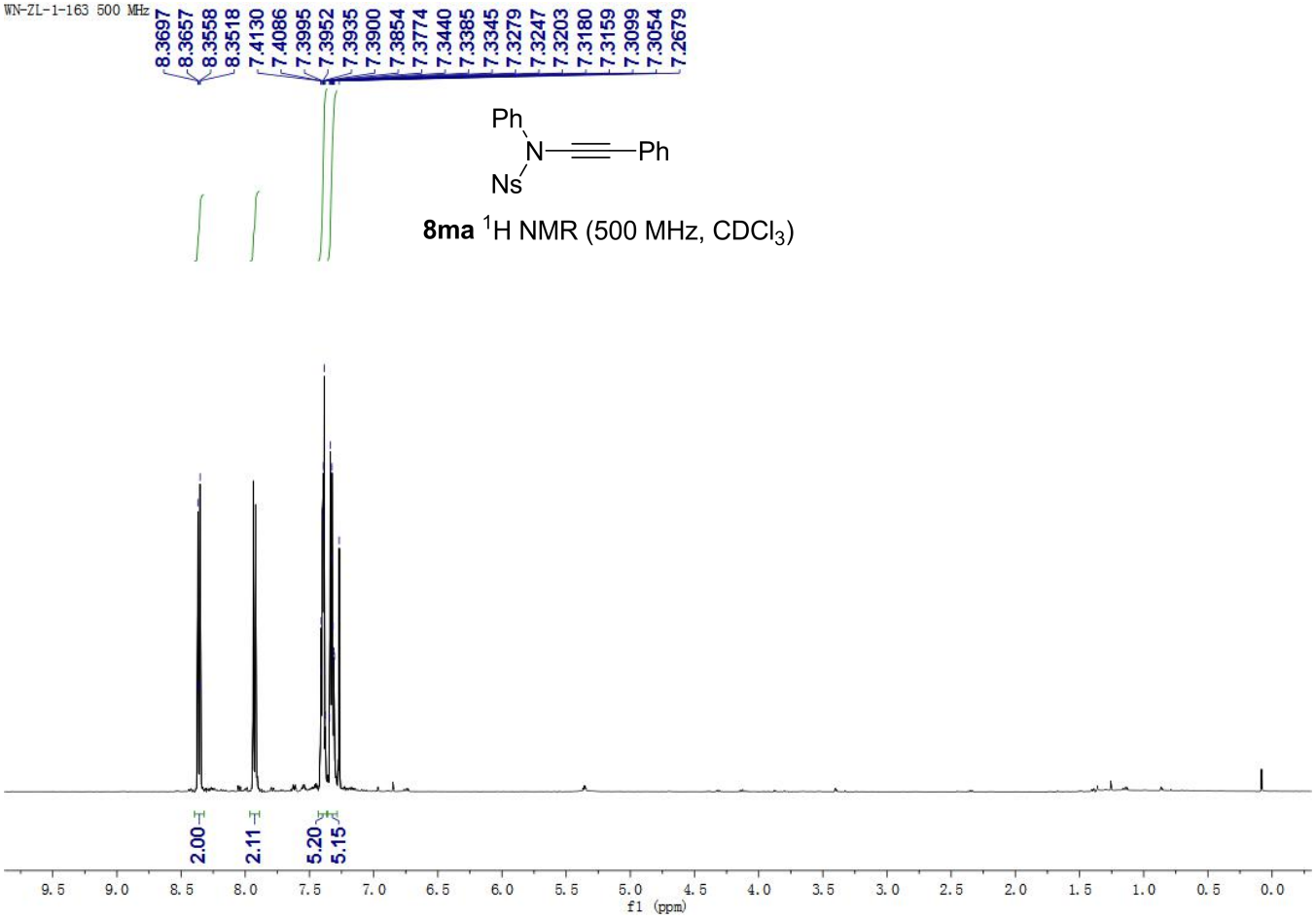

i-Pr
Ts
N
H
Ph
8ka $^{13}$C{$^{1}$H} NMR (125 MHz, $d_6$-acetone)
f1 (ppm)



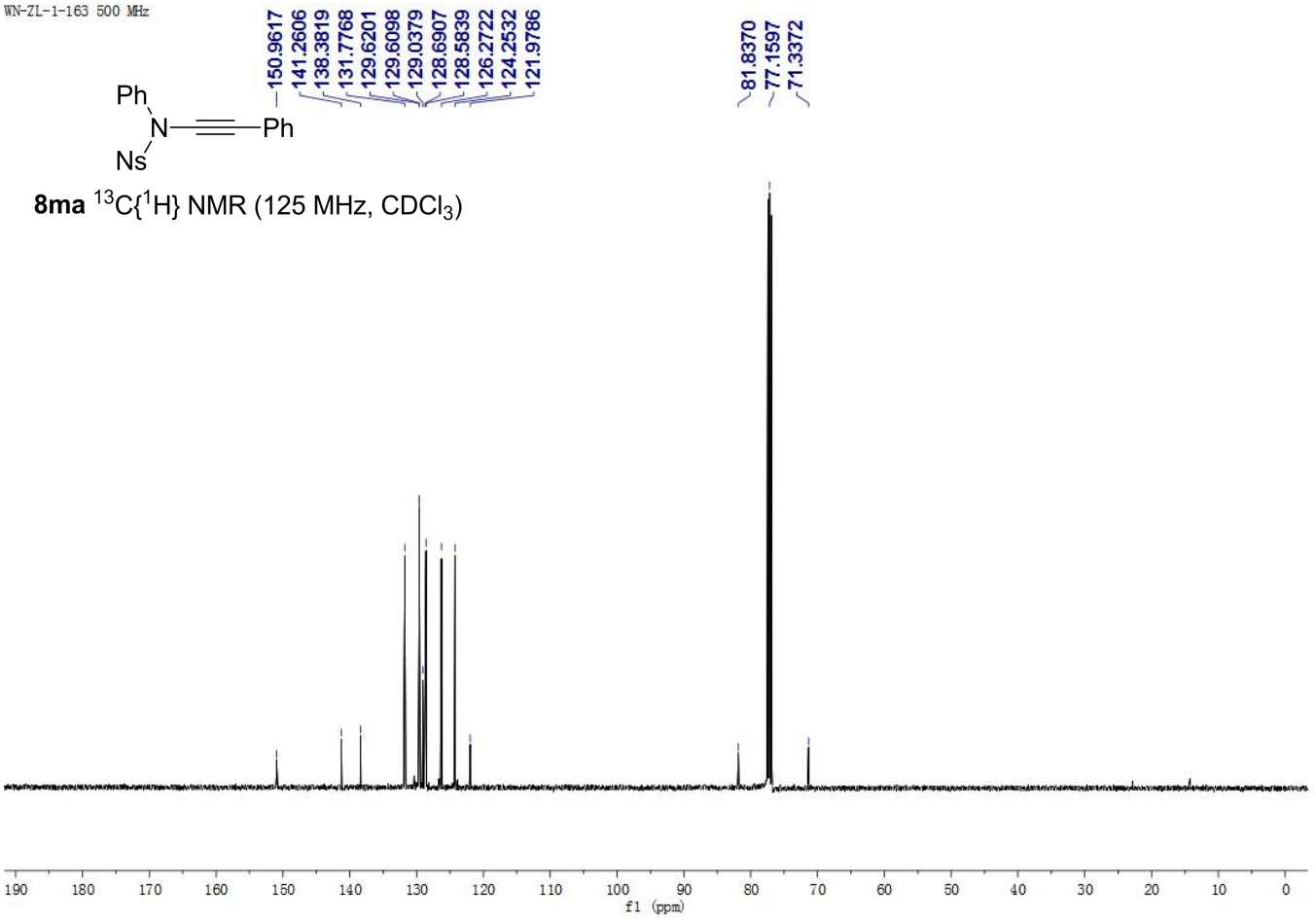

**8la** $^{1}$H NMR (400 MHz, $d_6$-acetone)



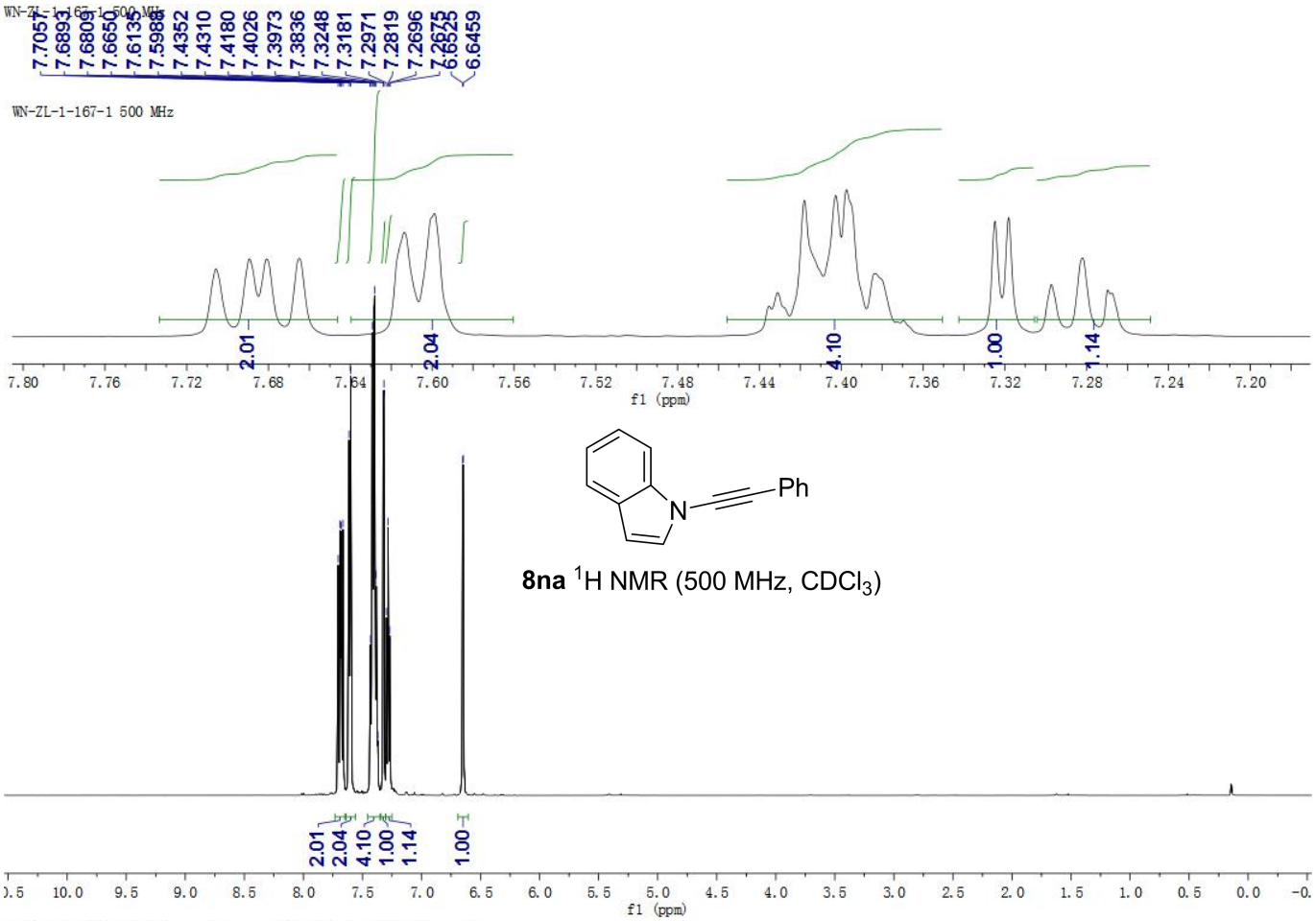

**8la** $^{13}$C{$^{1}$H} NMR (100 MHz, $d_6$-acetone)



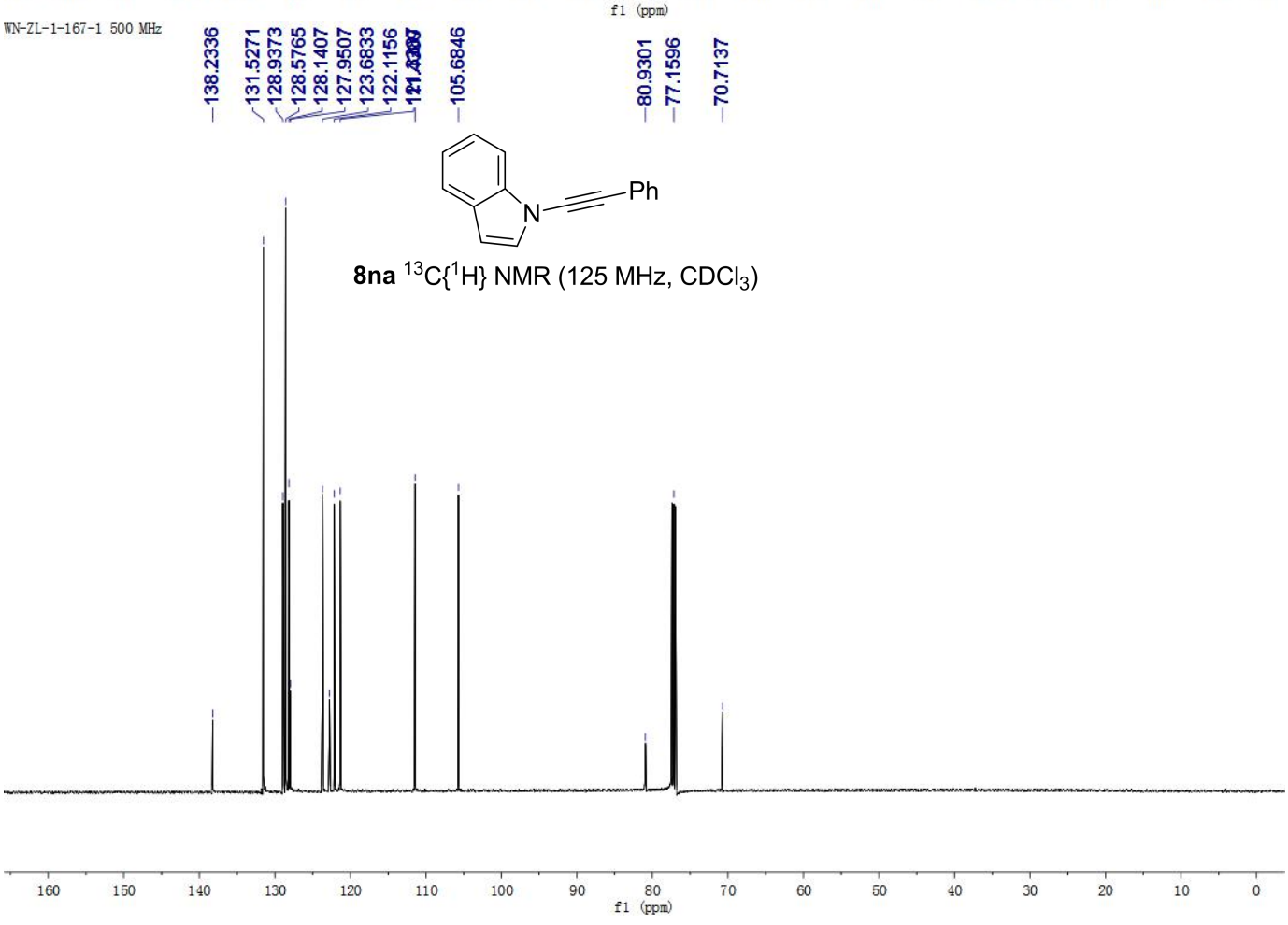

**8ma** $^{1}$H NMR (500 MHz, $CDCl_3$)



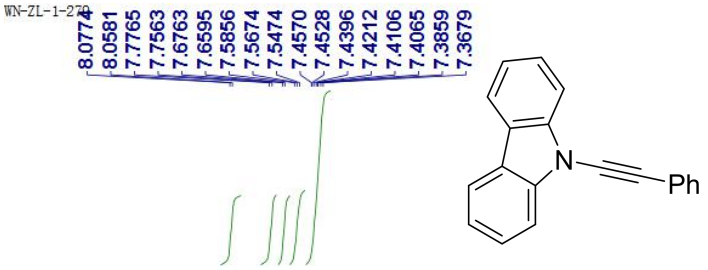

**8ma** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)



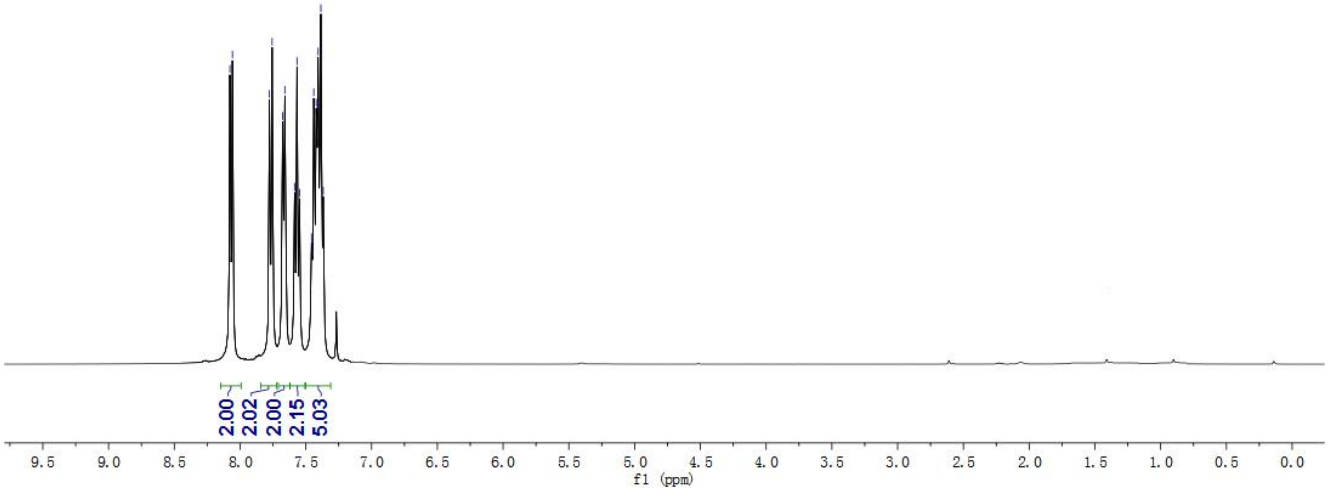

**8na** $^{1}$H NMR (500 MHz, $CDCl_3$)

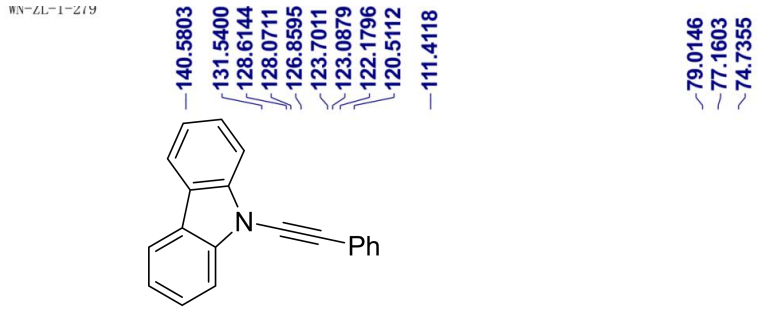



**8na** $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)

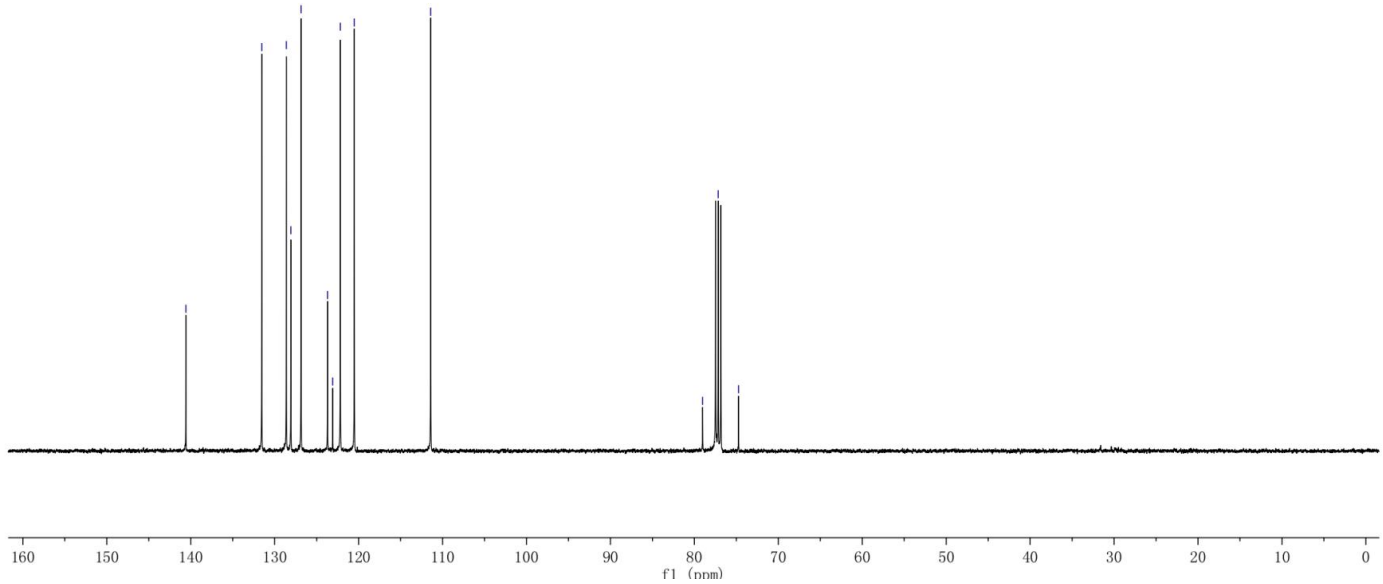


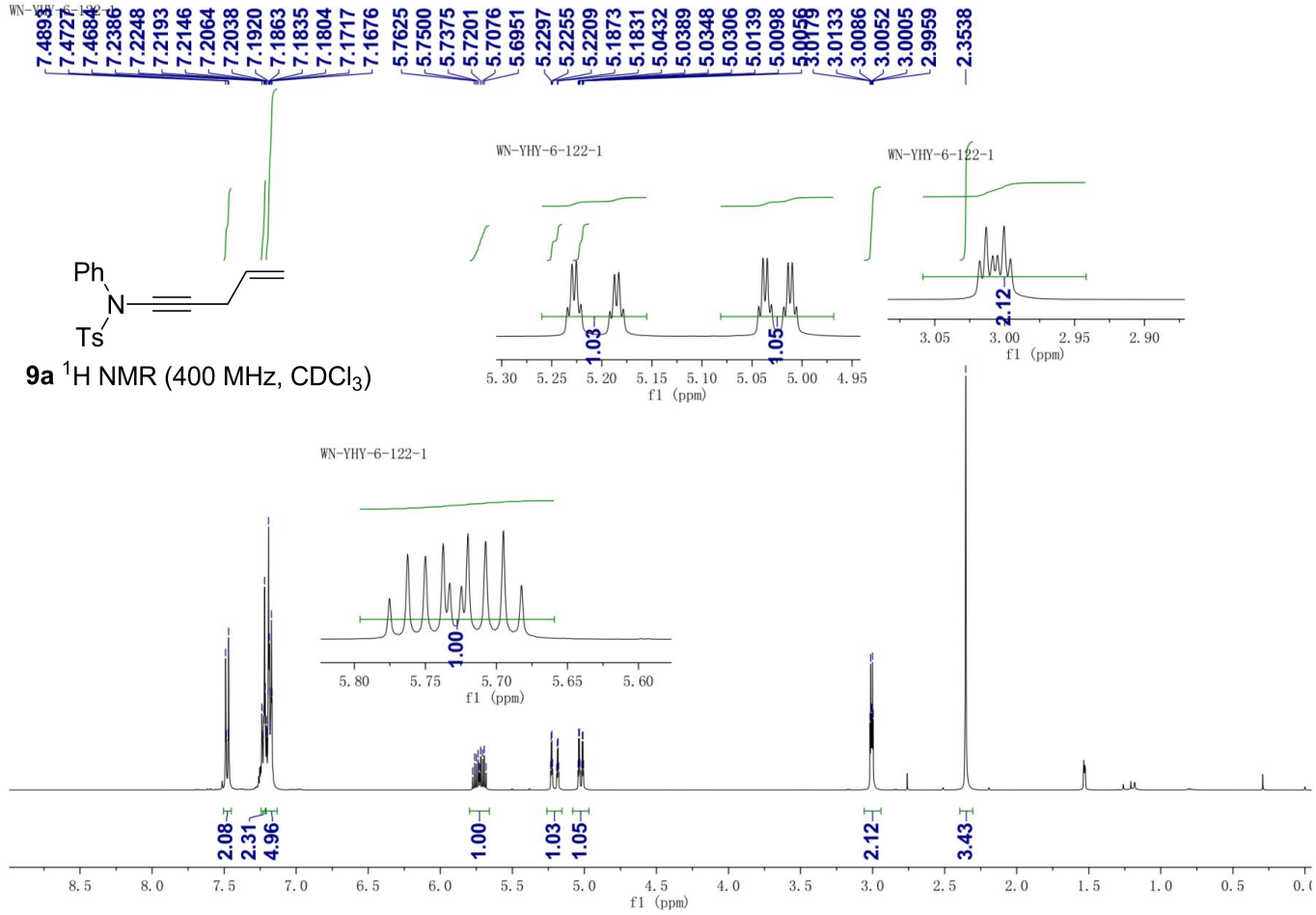

**8oa** $^{1}$H NMR (400 MHz, $CDCl_3$)



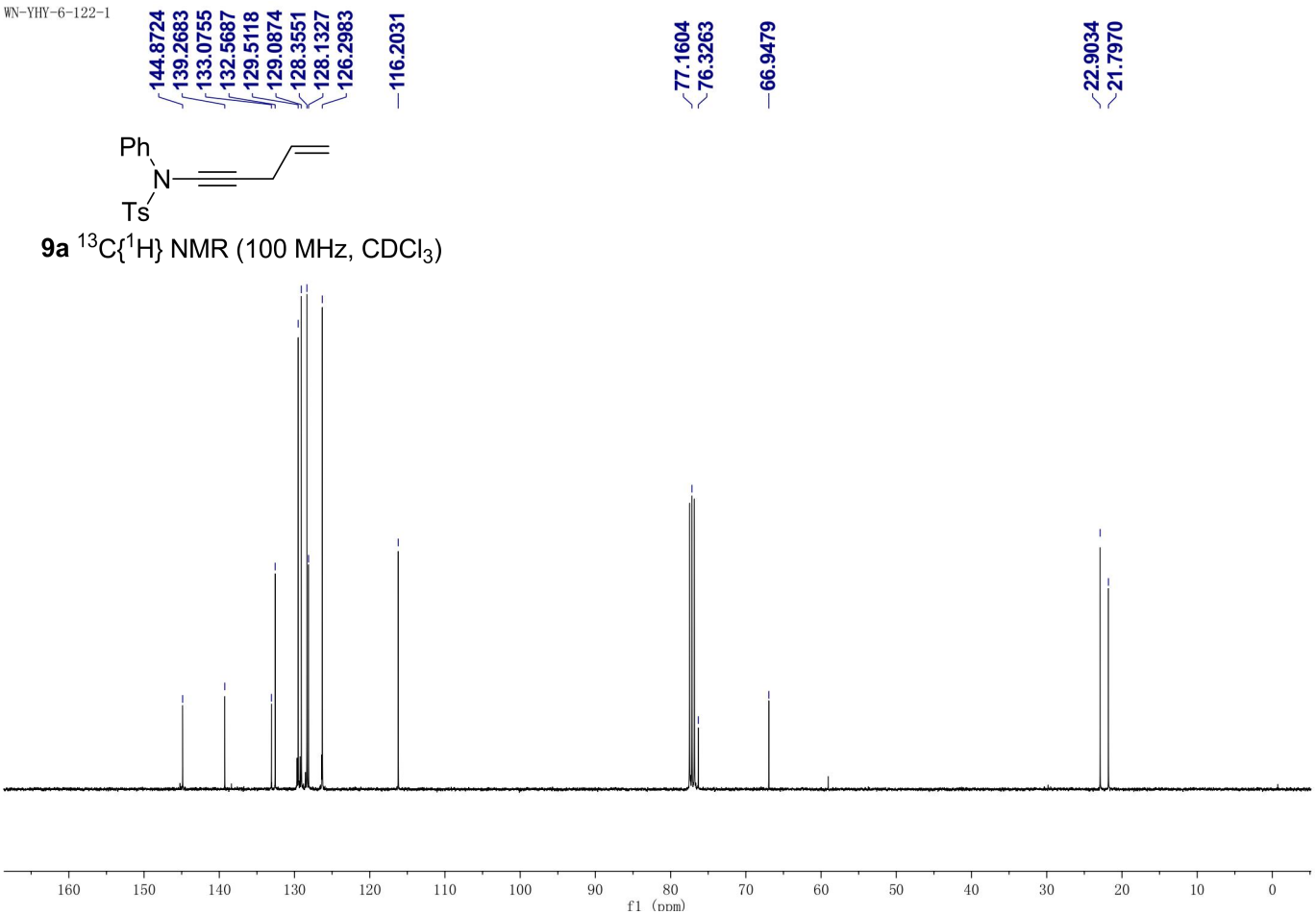




**8oa** $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

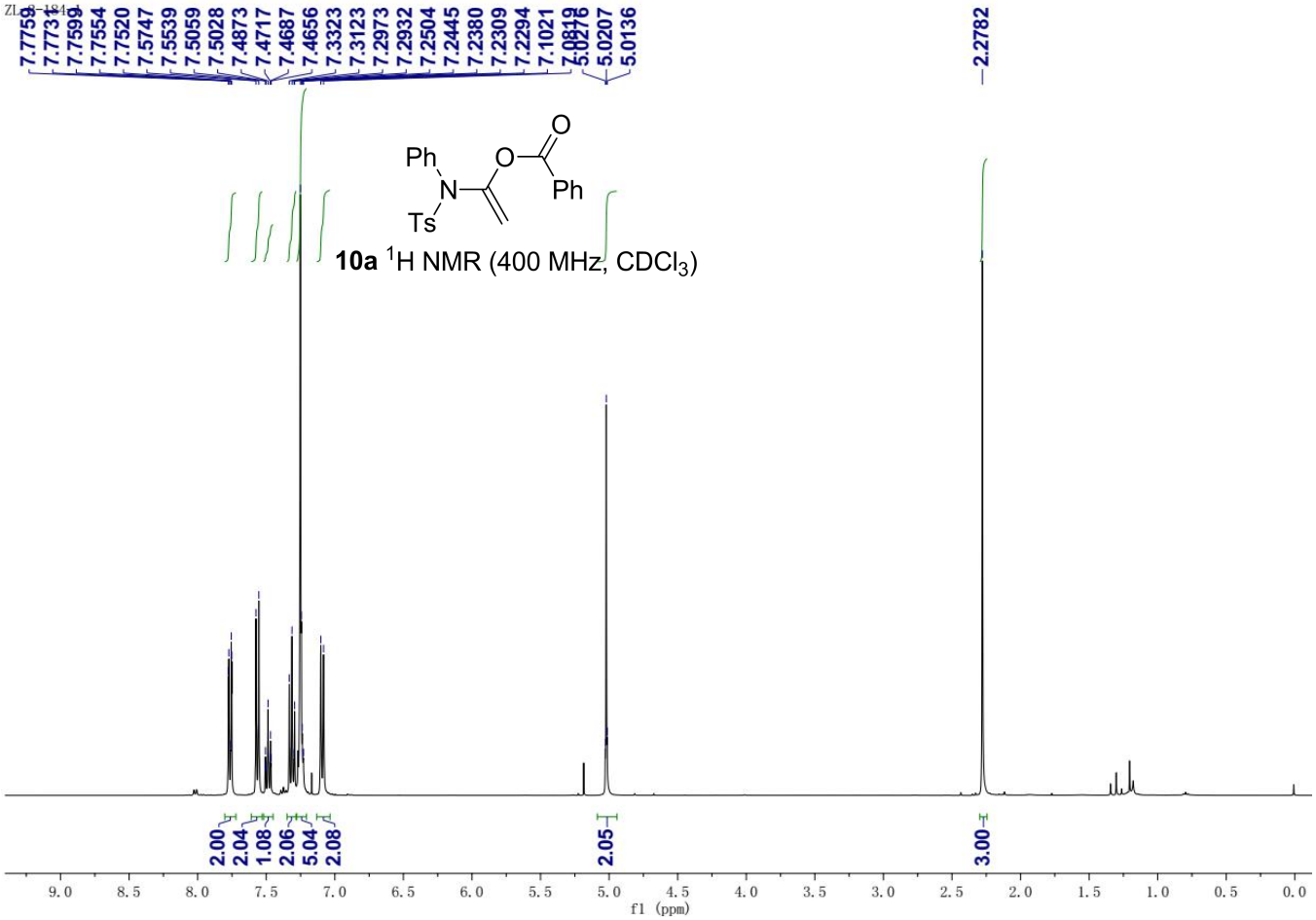




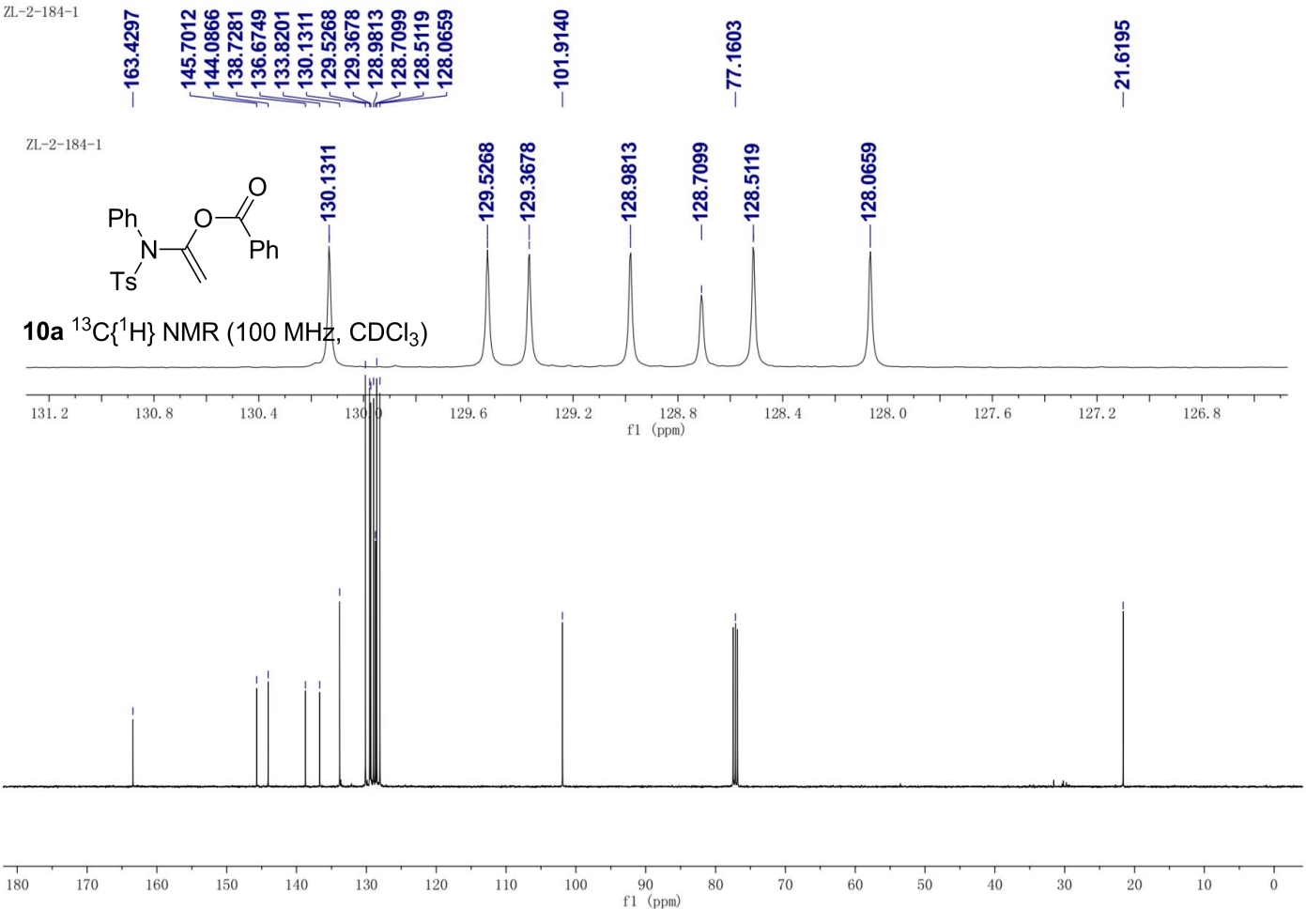

**9a** $^{1}$H NMR (400 MHz, $CDCl_3$)



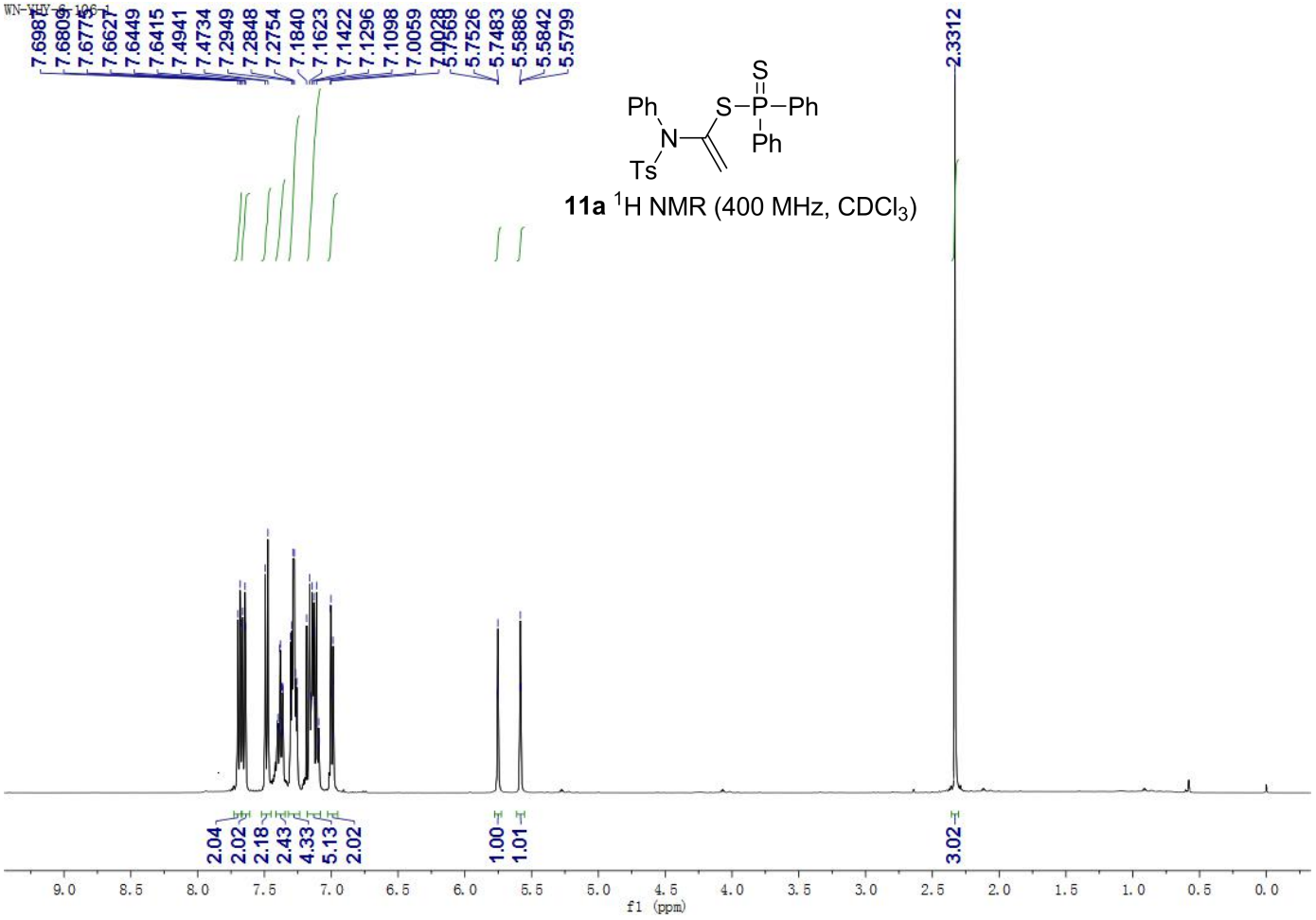

**9a** $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



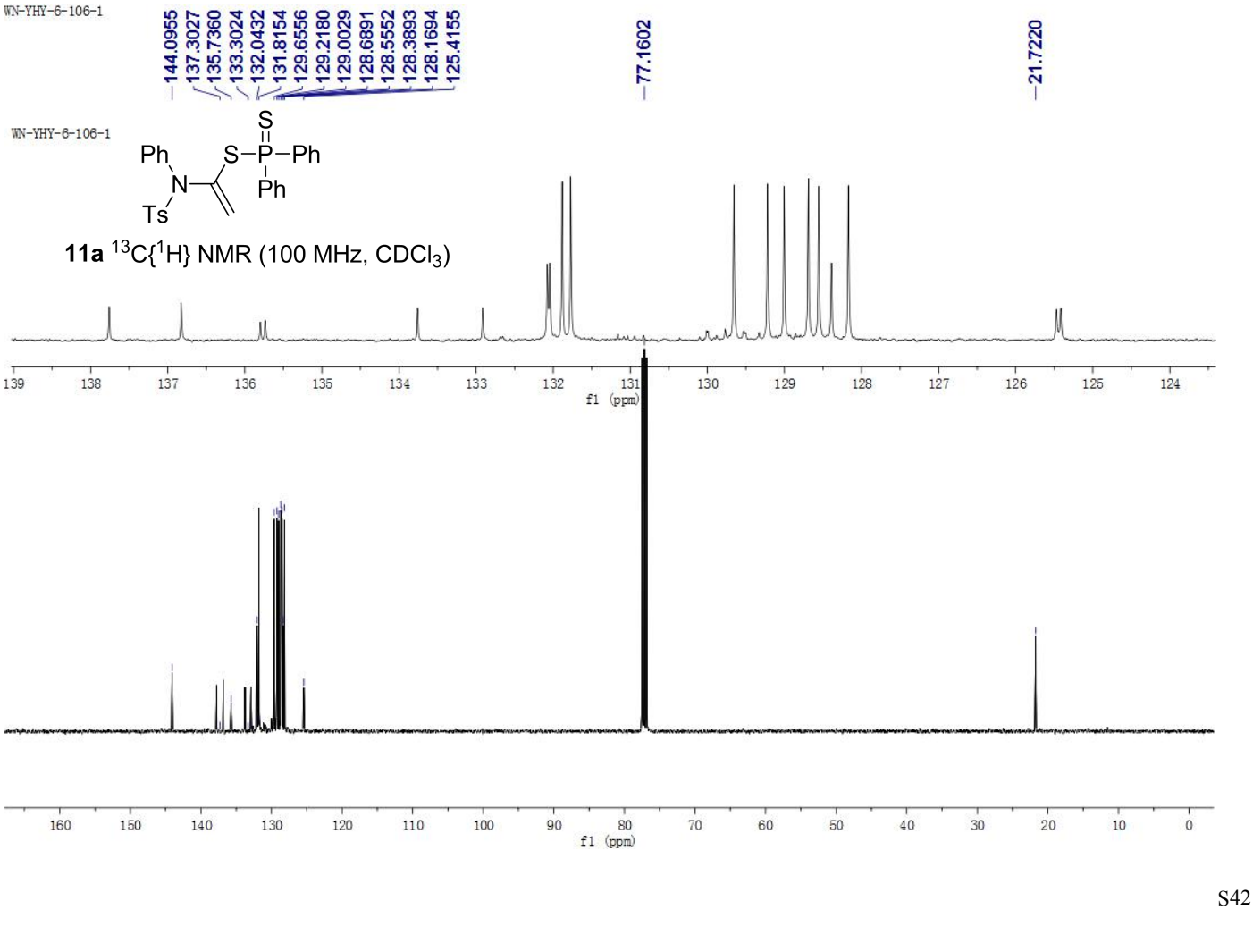

**10a** $^{1}$H NMR (400 MHz, $CDCl_3$)




**10a** $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

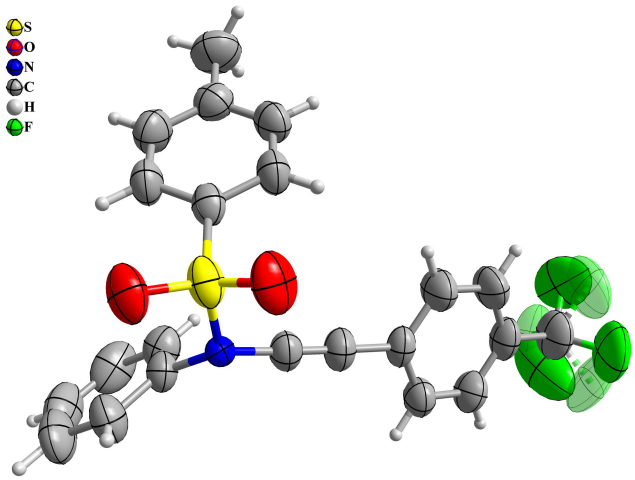



**11a** $^{1}$H NMR (400 MHz, $CDCl_3$)




**11a** $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

## 2. X-ray crystal structure of 8aj




ORTEP drawing of **8aj** showing thermal ellipsoids at the 50% probability level.

Crystal evaluation and data collection were performed at room temperature on a Bruker APEX2 CCD area detector diffractometer using graphite monochromated Mo-Kα radiation (λ = 0.71073 Å, sealed X-ray tube. Using Olex2,[1] the structure was solved with the ShelXS[2] structure solution program using charge flipping and refined with the ShelXL[3] refinement package using least-squares minimization. All nonhydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms on the structure were placed in idealized positions and refined using a riding model. The detailed crystallographic data and structure refinement parameters were summarized in Table S1. Selected bond lengths for compound **8aj** were collected in Table S2. Crystallographic data for the structural analyses has been deposited at the Cambridge Crystallographic Data Centre (CCDC reference numbers:1890688).
White prisms; m.p. 151.8 -152.6 ℃; recrystalised in ethyl acetate and petroleum ether.

**Table S1.** Crystallographic data and structure refinement parameters of **8aj**

| **Identification code** | **8aj** |
|---|---|
| Empirical formula | $C_{22}H_{16}F_3N_3O_2S$ |
| Formula weight (M) | 415.42 |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a (Å) | 13.923(4) |
| b (Å) | 8.463(2) |
| c (Å) | 18.232(5) |
| *a* (°) | 90 |
| *β* (°) | 109.888(4) |
| *g* (°) | 90 |
| V/( Å $^3$) | 2020.0(9) |

| | |
|---|---|
| Z | 4 |
| Dc( Mg m-3) | 1.366 |
| F(000) | 856 |
| Reflections collected | 23039 / 4137 |
| unique | R(int) = 0.0459 |
| Goodness-of-fit on F2 | 1.037 |
| Final R indices | R1 = 0.0432 |
| I > 2σ(I) | ωR2 = 0.1187 |
| R indices | R1 = 0.0667 |
| (all data) | ωR2 = 0.1358 |

**Table S2** Selected bond length for **8aj**

**1 .**

**Atomic Distances**

**[Å]**

| | | | |
|---|---|---|---|
| S1—O1 | 1.4279 (15) | C8—F3' | 1.261 (12) |
| S1—O2 | 1.4216 (15) | C8—F2' | 1.308 (13) |
| S1—N1 | 1.6909 (18) | C8—F1' | 1.29 (2) |
| S1—C5 | 1.742 (2) | C9—C10 | 1.379 (3) |
| N1—C16 | 1.370 (2) | C9—C14 | 1.372 (3) |
| N1—C17 | 1.454 (2) | C10—C11 | 1.373 (3) |
| C1—C2 | 1.501 (3) | C11—C12 | 1.390 (3) |
| C2—C3 | 1.384 (3) | C12—C13 | 1.375 (3) |
| C2—C7 | 1.379 (3) | C12—C15 | 1.442 (3) |
| C3—C4 | 1.373 (3) | C13—C14 | 1.379 (3) |
| C4—C5 | 1.386 (3) | C15—C16 | 1.180 (3) |
| C5—C6 | 1.392 (3) | C17—C18 | 1.380 (3) |
| C6—C7 | 1.373 (3) | C17—C22 | 1.372 (3) |
| C8—C9 | 1.491 (3) | C18—C19 | 1.379 (3) |
| C8—F1 | 1.295 (8) | C19—C20 | 1.354 (4) |
| C8—F2 | 1.342 (6) | C20—C21 | 1.371 (4) |

| | | | |
|---|---|---|---|
| C8—F3 | 1.323 (6) | C21—C22 | 1.384 (4) |

3. **Reference**:

(1) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX$^2$: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **2009**, *42*, 339-341.
(2) Sheldrick, G. M. A short history of SHELX. *Acta. Crystallogr. A*. **2008**, *A64*, 112-122.
(3) Sheldrick, G. M. Crystal structure refinement with SHELXL. *Acta. Crystallogr. C*. **2015**, *C71*, 3-8.