Supporting Information

Pd-catalyzed Multicomponent Cascade Protocols to β-Indolyl Sulfoximidoyl Amides via Intermolecular Trapping of α-Indolylpalladium Complex by CO

Huahua Liu, Li Wei, and Zhiyuan Chen*

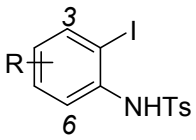
Key Laboratory of Functional Small Organic Molecules, Ministry of Education and Jiangxi Key Laboratory of Green Chemistry, College of Chemistry & Chemical Engineering, Jiangxi Normal University, 99Ziyang Road, Nanchang, Jiangxi 330022 (P. R. China).

E-mail: zchen@jxnu.edu.cn

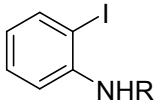
Contents

1. The substrates employed in this study (**S2**)
2. **^{1}H** and **^{13}C NMR** spectra of all new compounds **4-6** (**S3-S36**)
3. **^{1}H** and **^{13}C NMR** Spectra of compound **8** (**S37**)
4. X-ray crystal structure of compound **4v** (**S38-S39**)

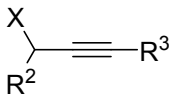
1. The substrates employed in this study.



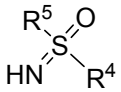
R = H, **1a**
R = 3-Cl, **1b**
R = 4-Me, **1c**
R = 4-MeO, **1d**
R = 4-F, **1e**
R = 4-Cl, **1f**
R = 5-Me, **1g**
R = 5-F, **1h**
R = 5-Cl, **1i**
R = 5-Br, **1j**
R = 4-CF_3, **1k**



R = Ac, **1l**
R = Boc, **1m**



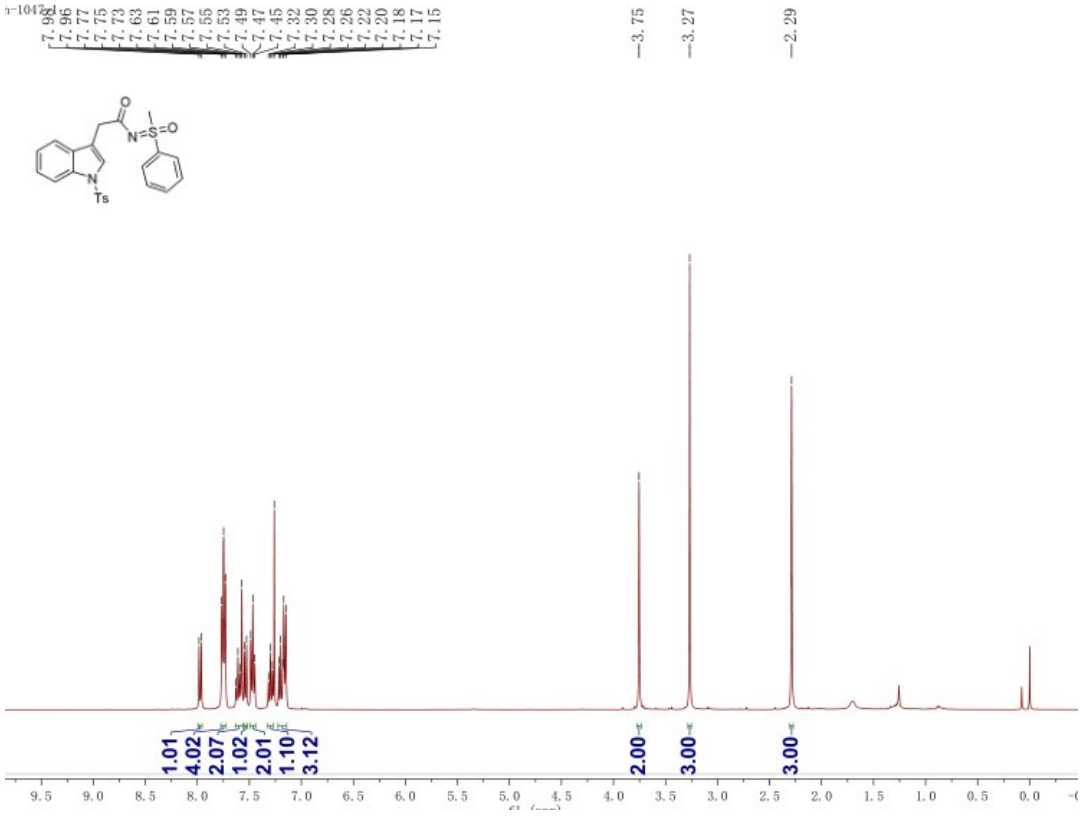
$R^2 = R^3$ = H, **2a**
$R^2 = R^3$ = Me, **2b**
$R^2 = R^3$ = Ph, **2c**
R^2 = H, R^3 = Ph, **2d**



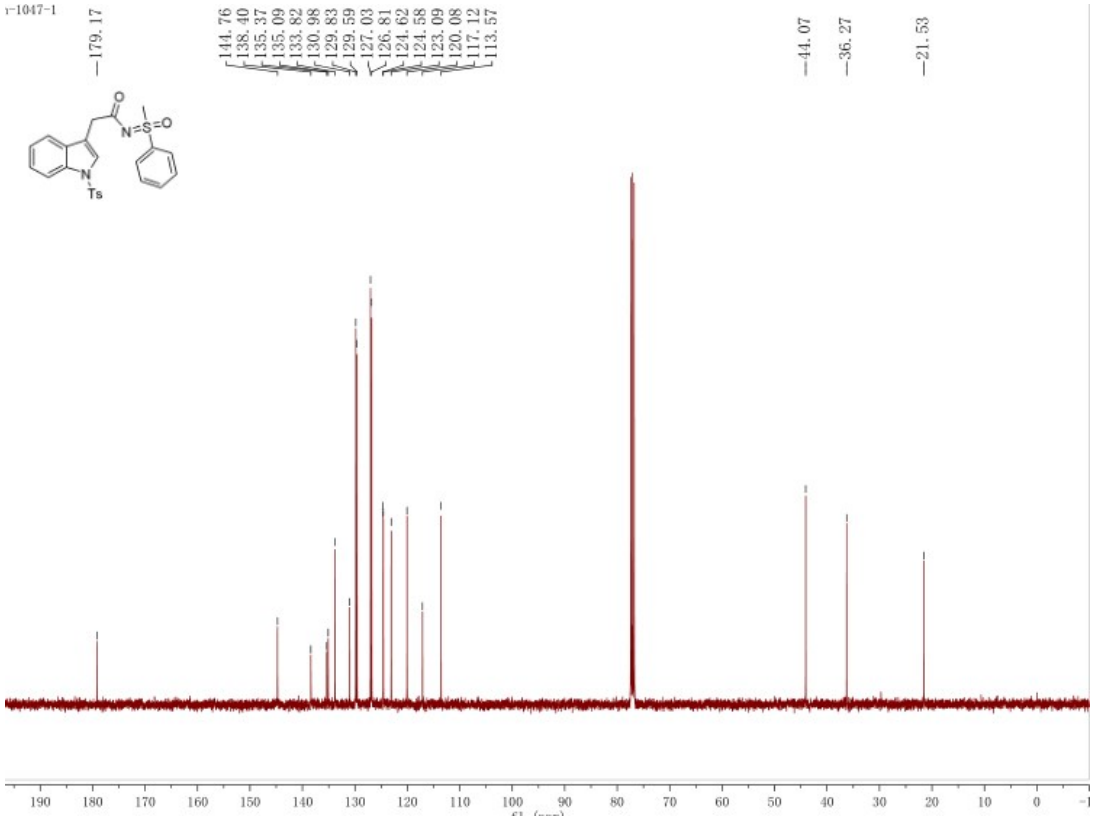
R^4 = Ph, R^5 = Me, **3a**
R^4 = Ph, R^5 = Et, **3b**
R^4 = Ph, R^5 = cyclopropyl, **3c**
R^4 = Ph, R^5 = Bn, **3d**
R^4 = 2-Naph, R^5 = Me, **3e**
R^4 = Ph, R^5 = Ph, **3f**
R^4 = Ph, R^5 = 4-MeC_6H_4, **3g**
$R^4 = R^5$ = 4-ClC_6H_4, **3h**
R^4 = 4-MeC_6H_4, R^5 = 4-BzC_6H_4, **3i**

2. ^{1}H and ^{13}C NMR Spectra of all new compounds 4-6.

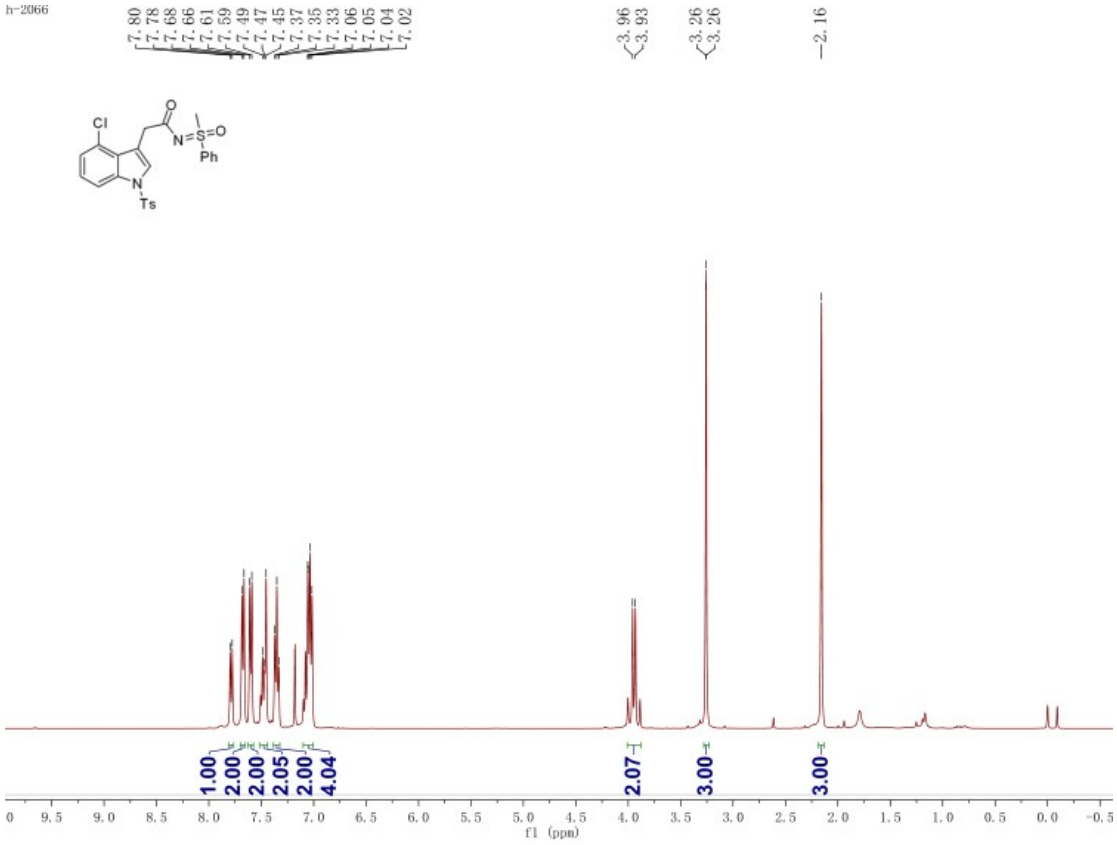
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4a.



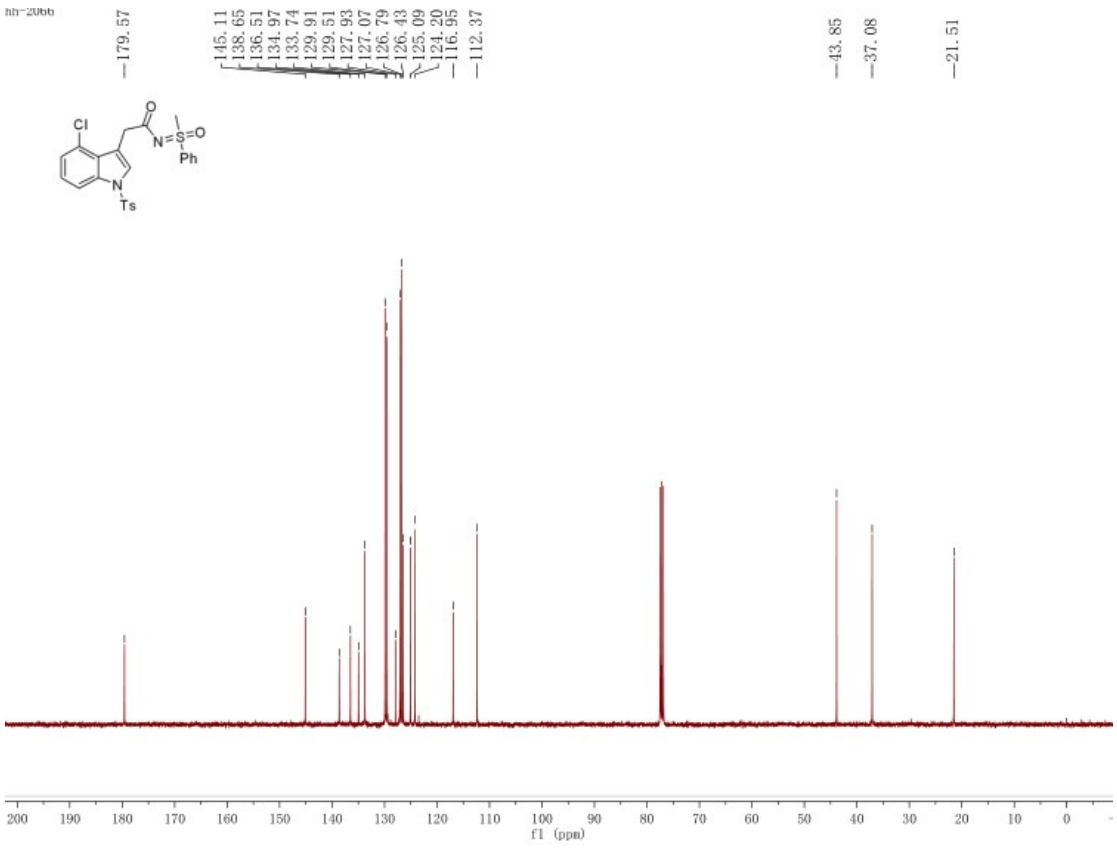
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4a



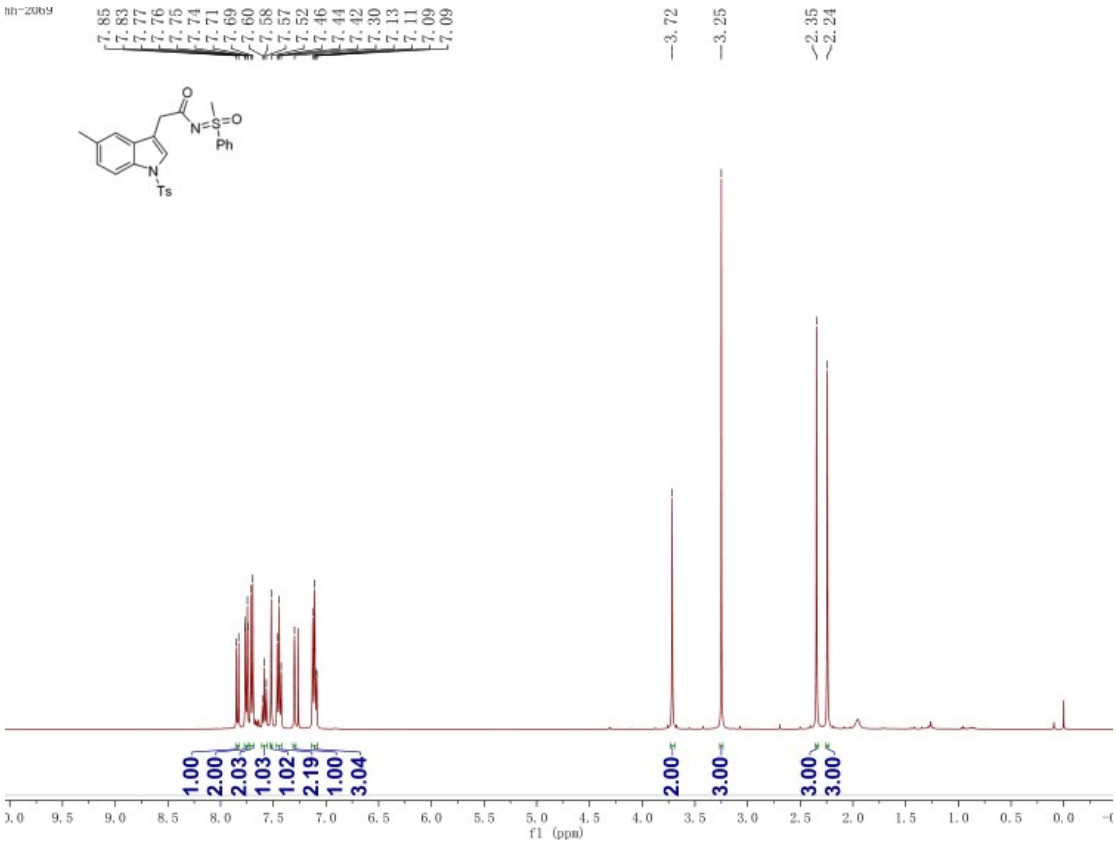
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4b



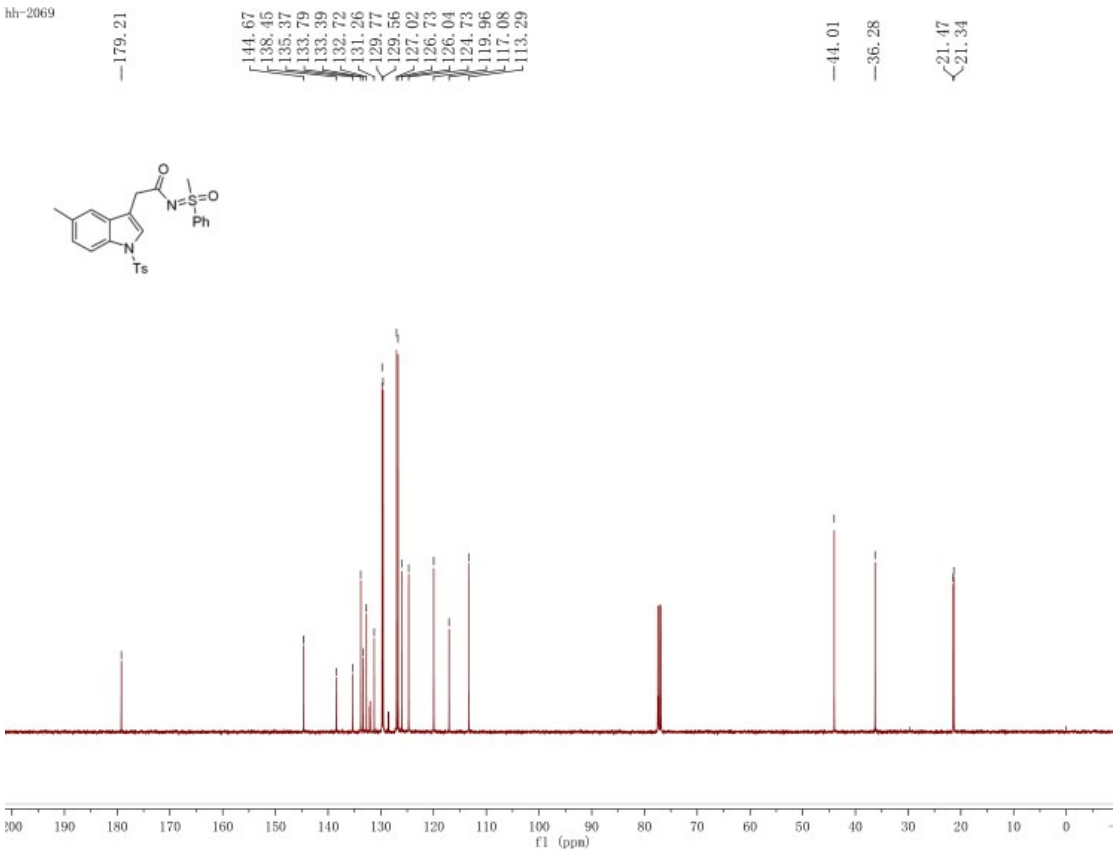
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4b



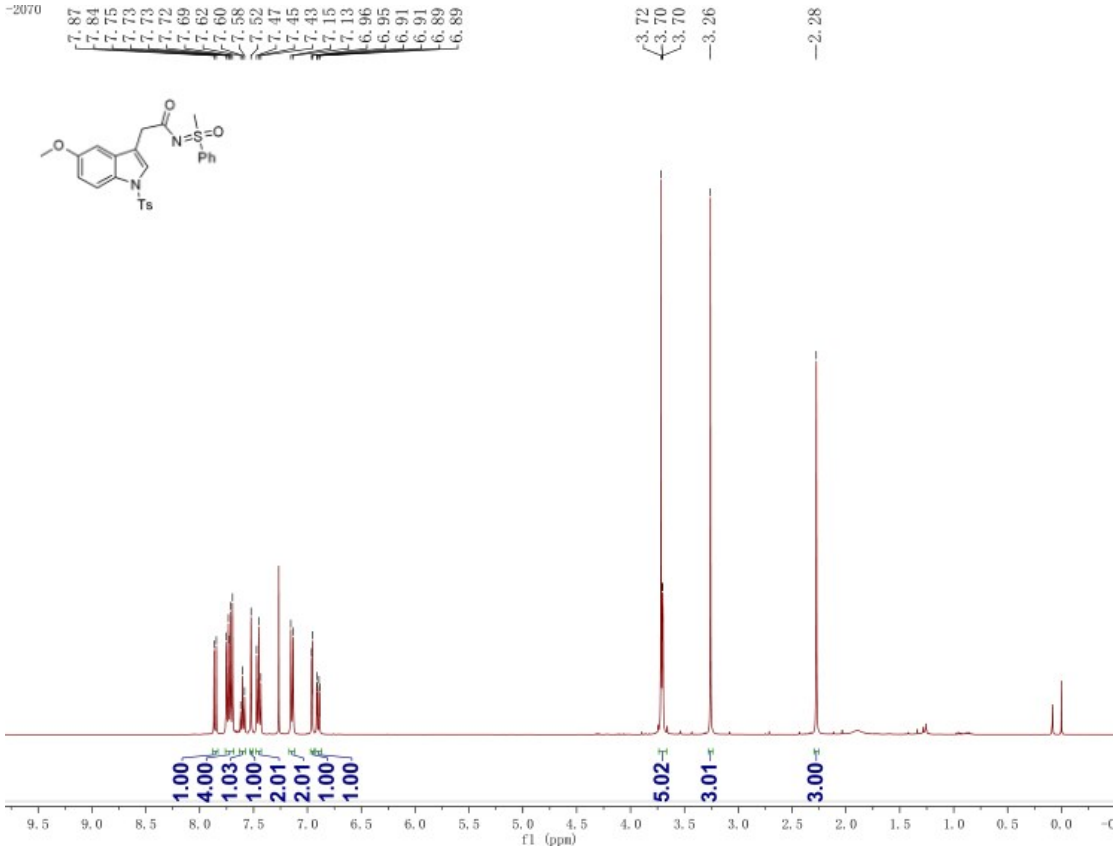
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4c



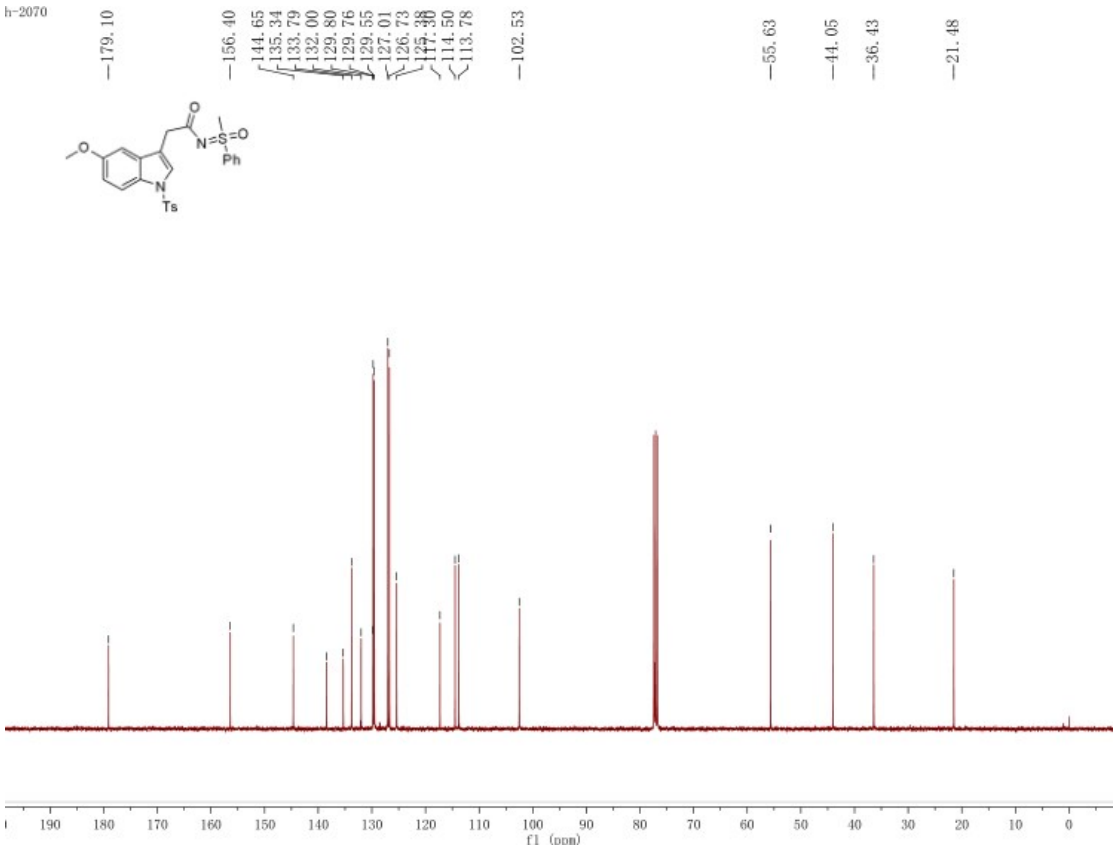
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4c



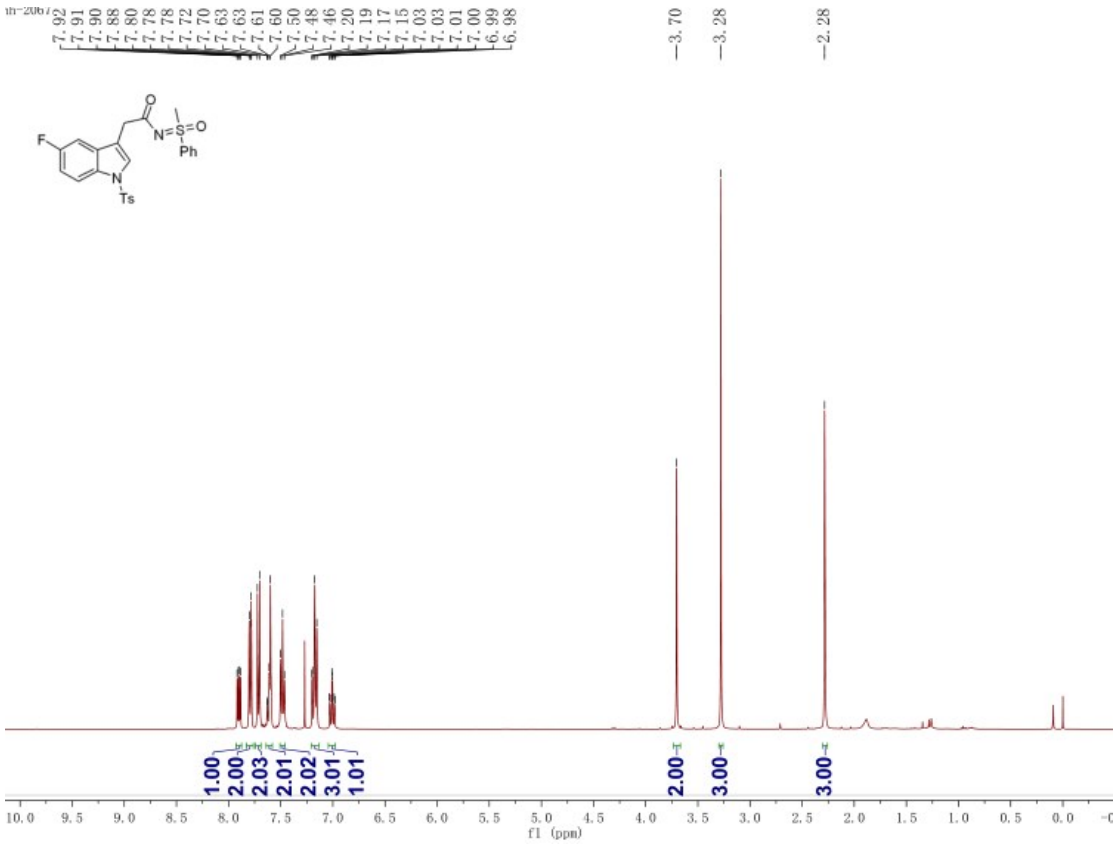
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4d



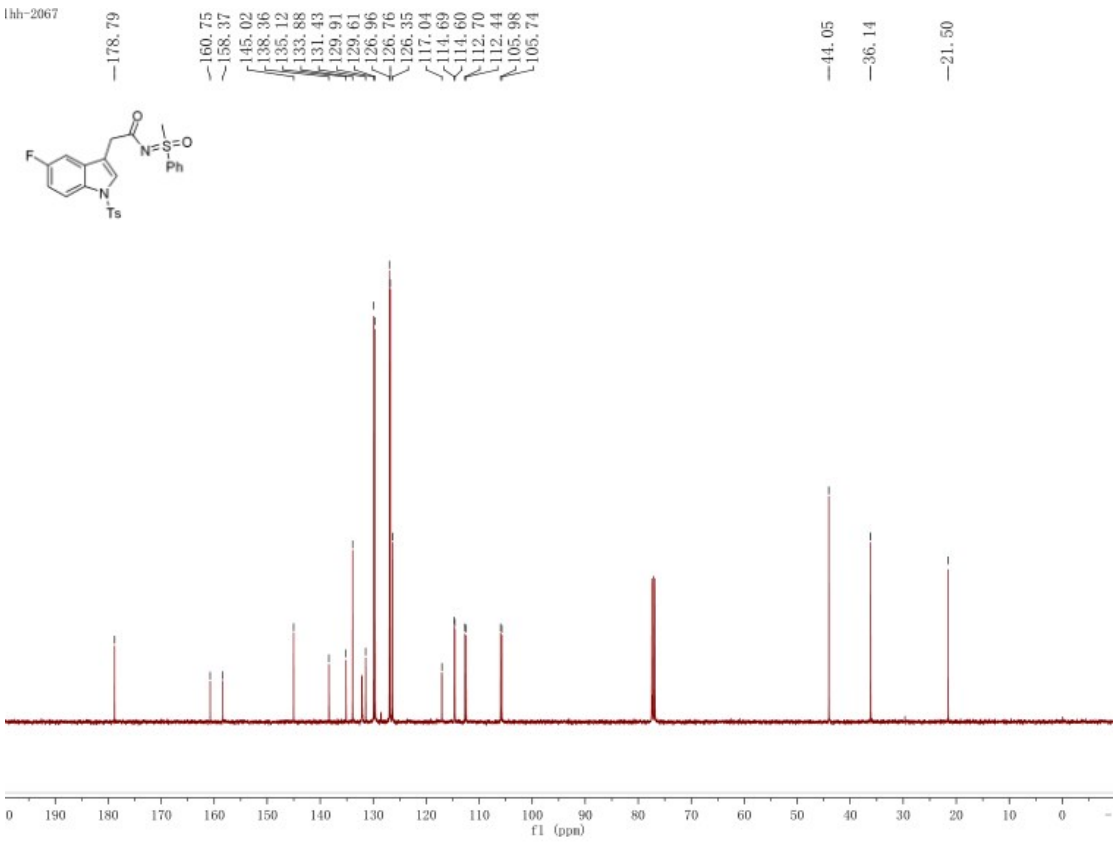
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4d



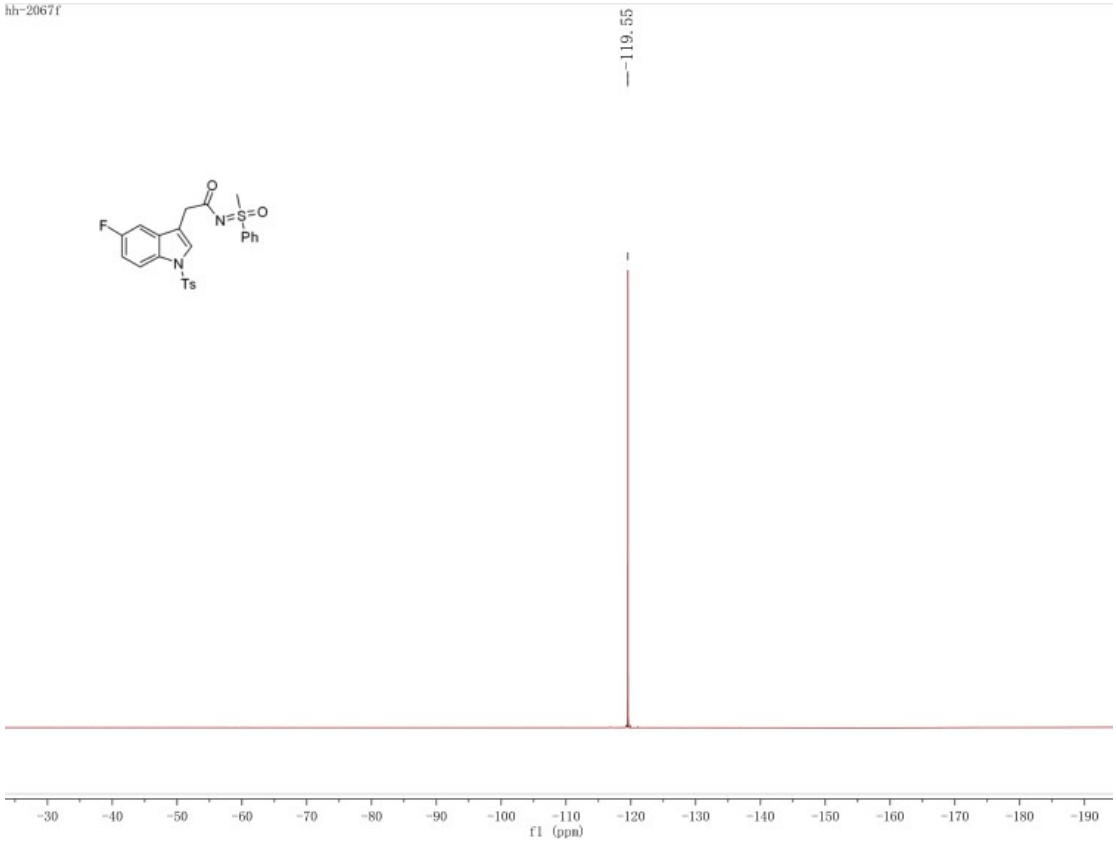
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4e



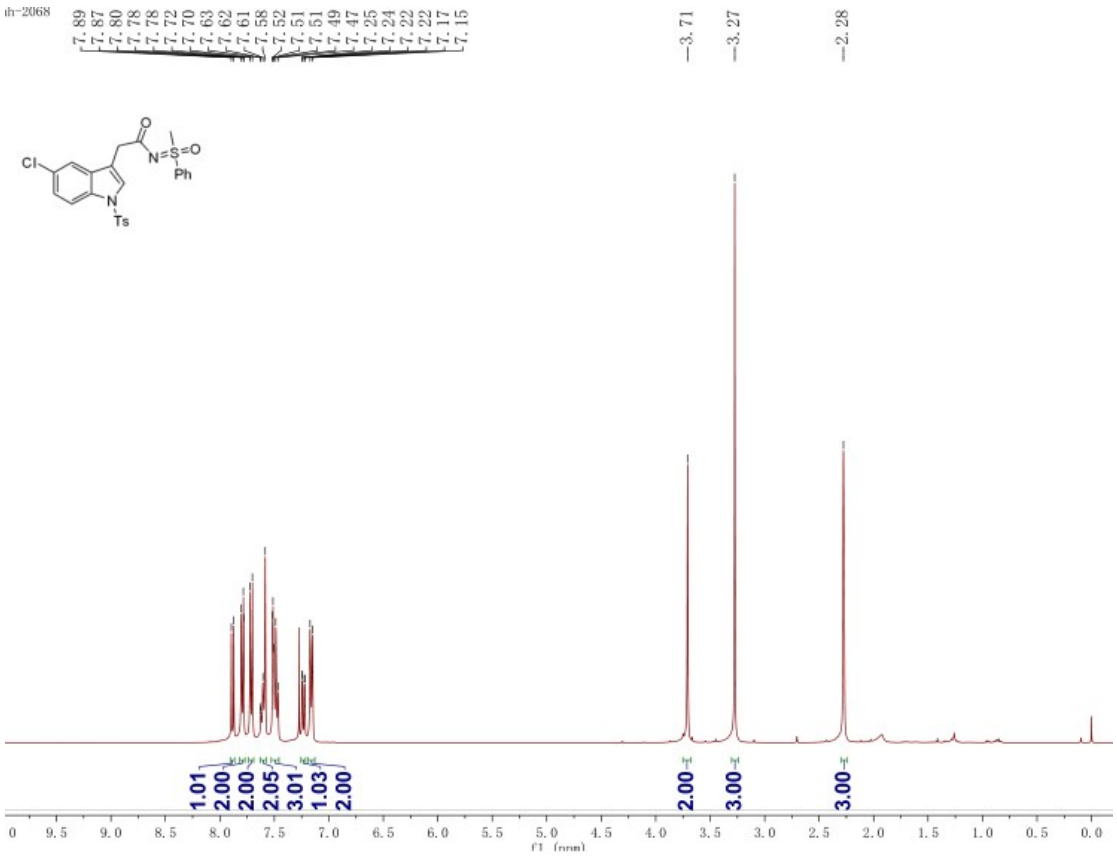
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4e



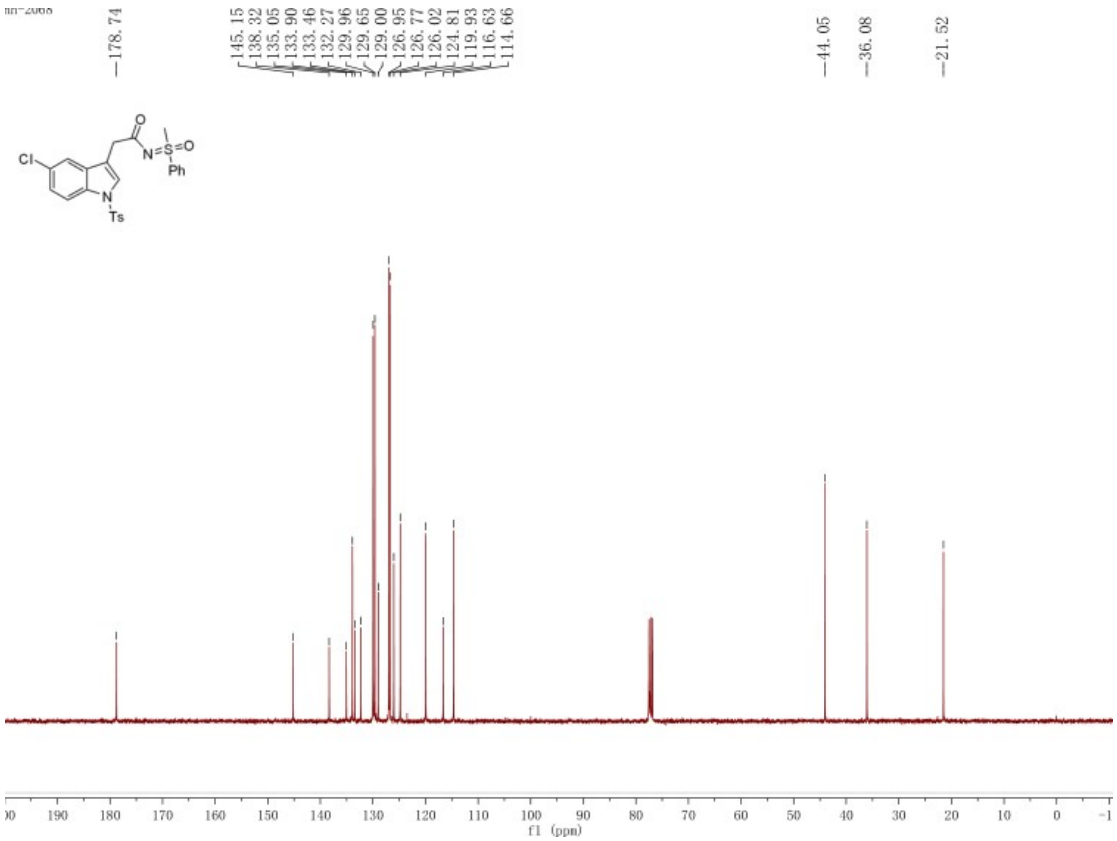
^{19}F NMR (376 MHz, $CDCl_3$) of 4e



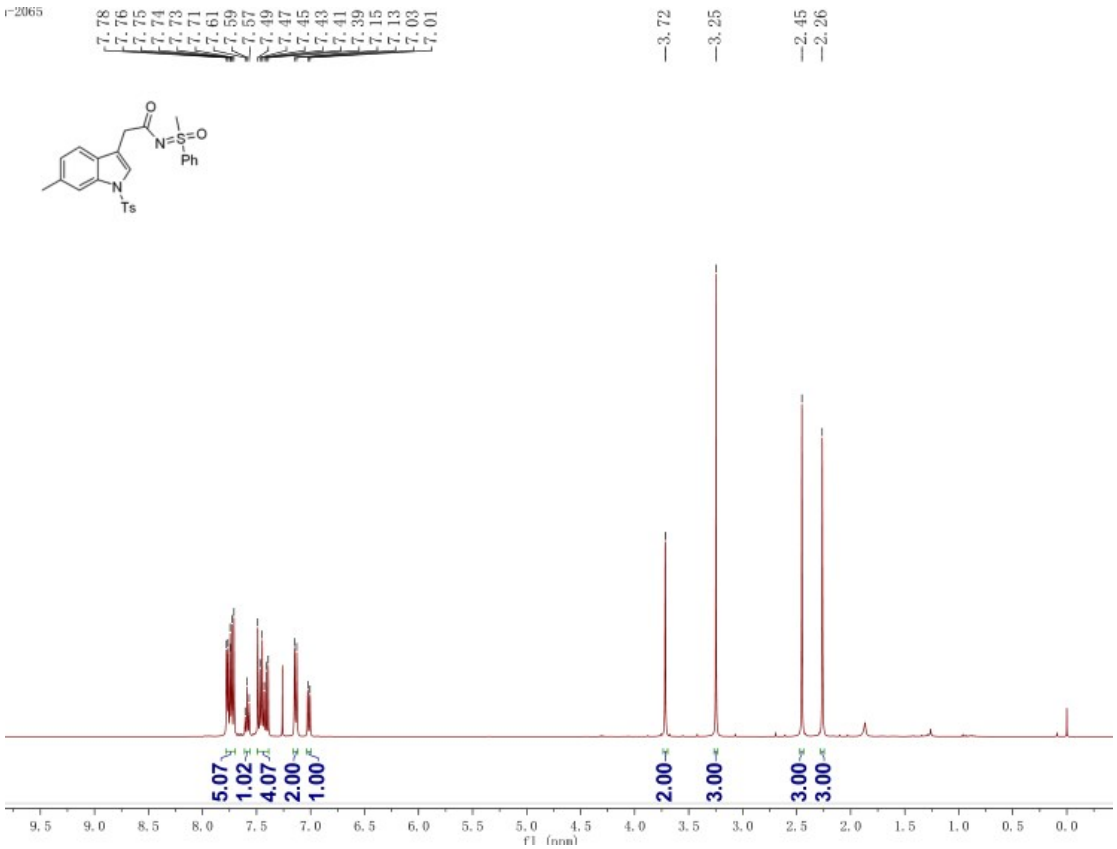
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4f



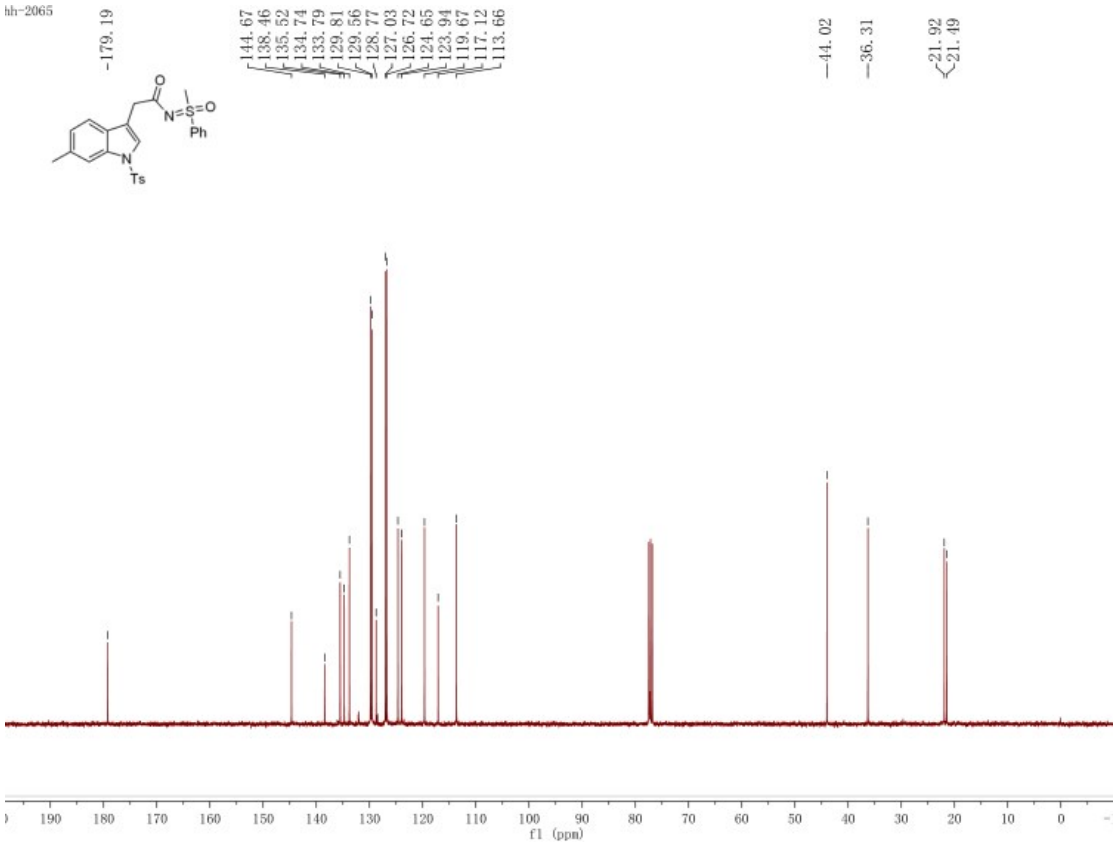
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4f



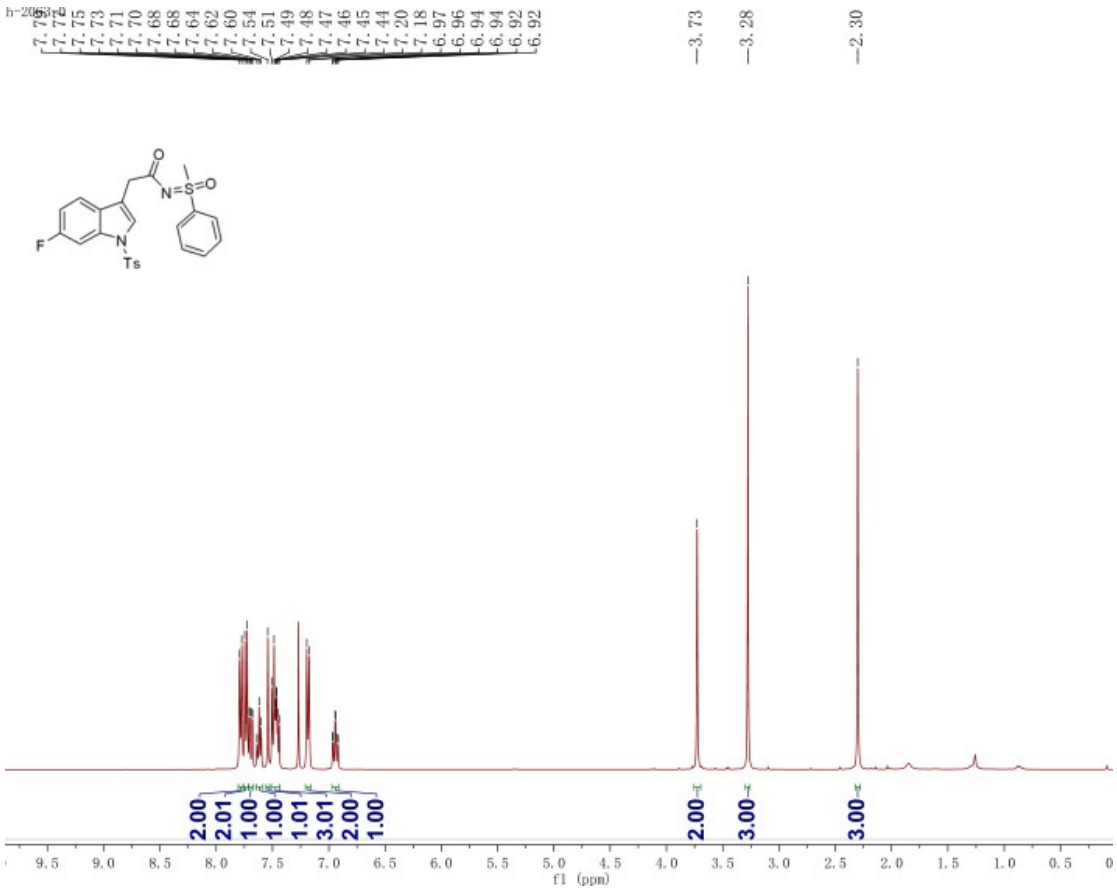
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4g



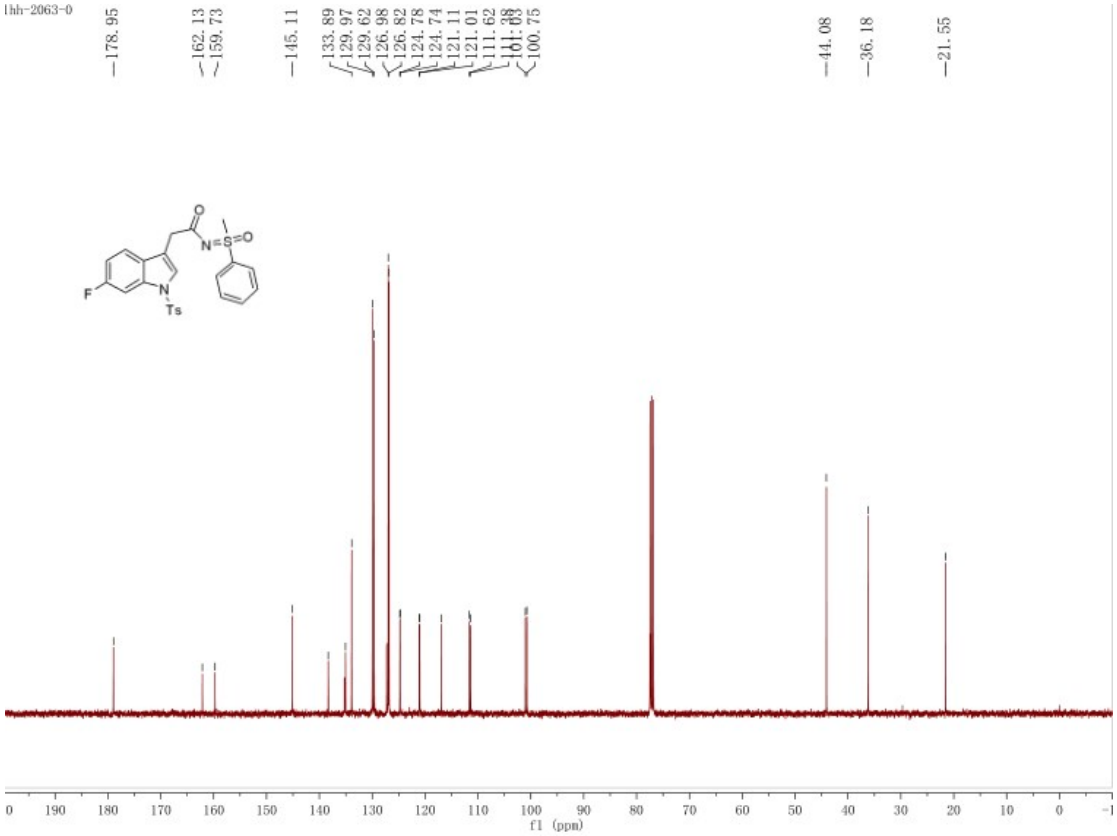
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4g



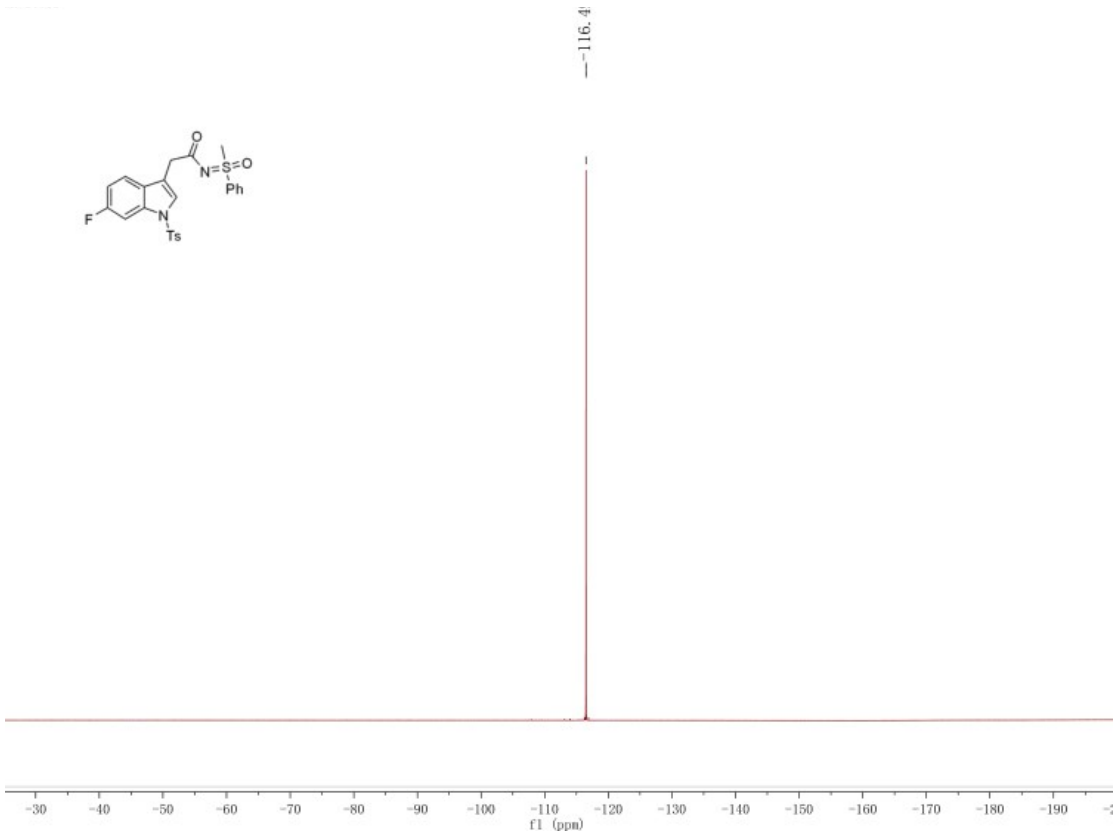
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4h



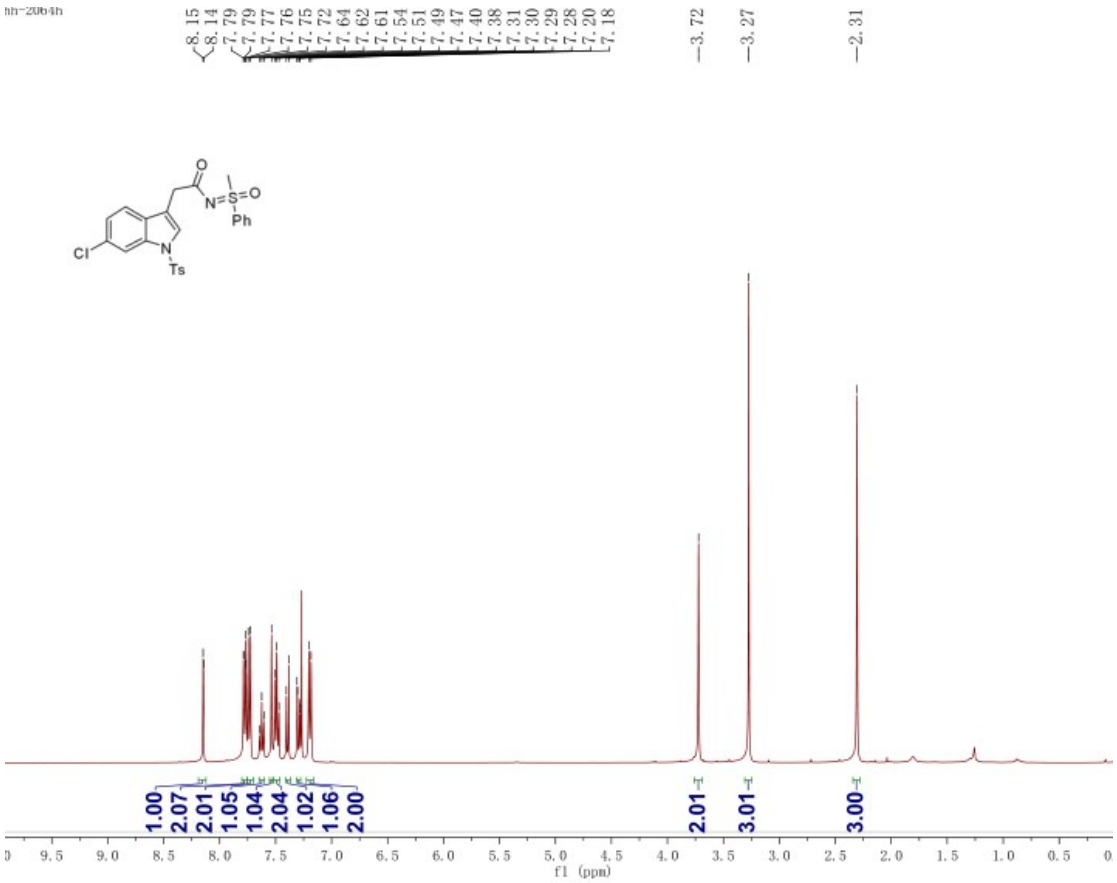
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4h



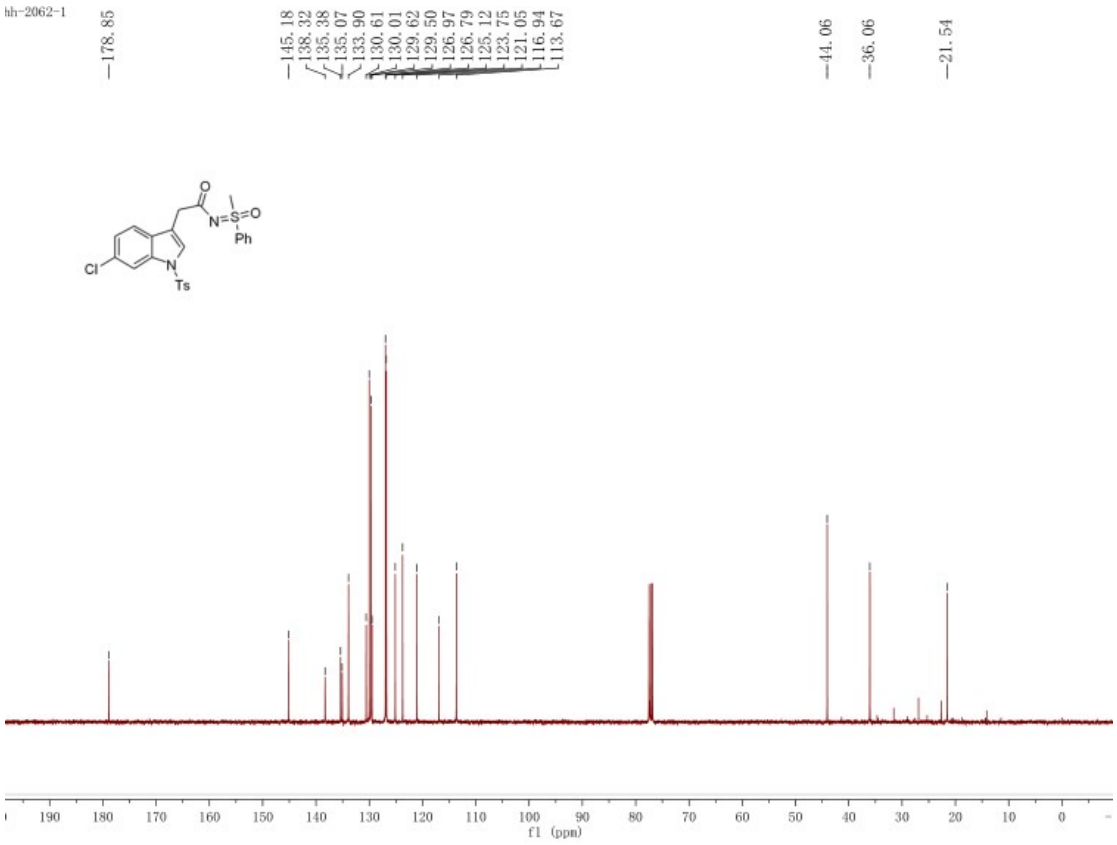
^{19}F NMR (376 MHz, $CDCl_3$) of 4h



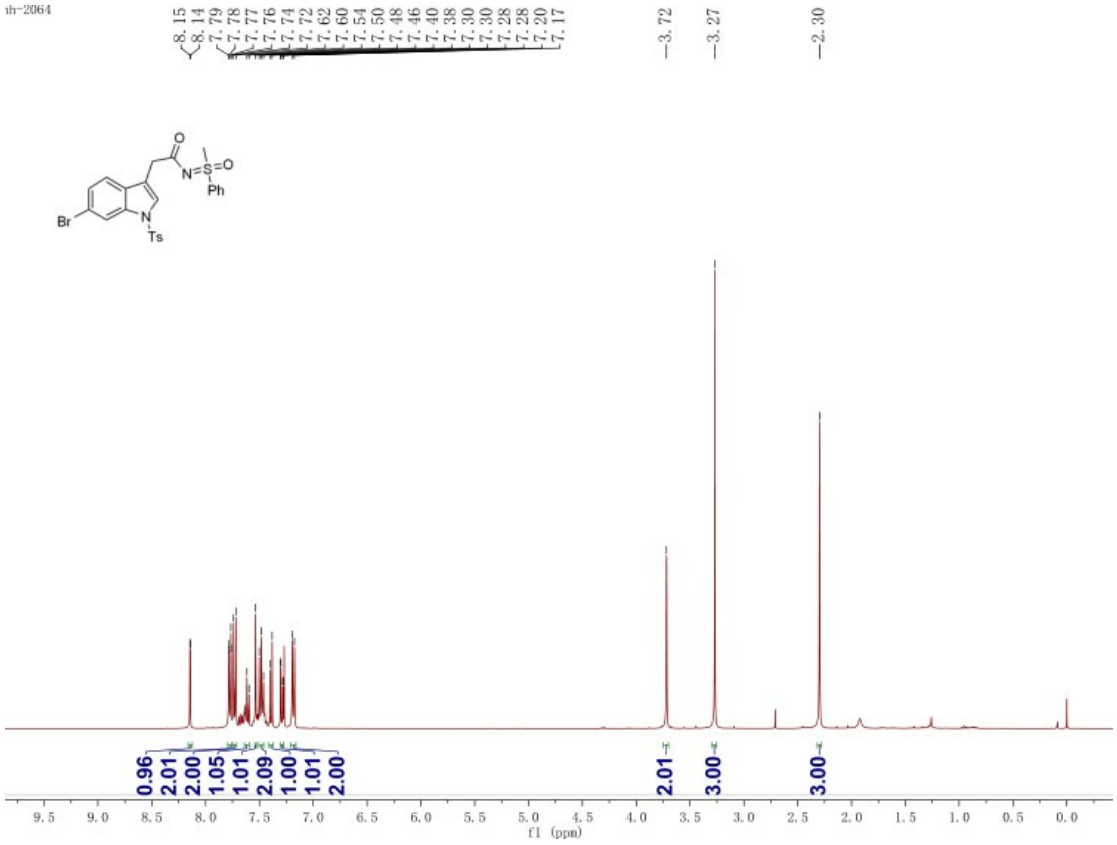
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4i



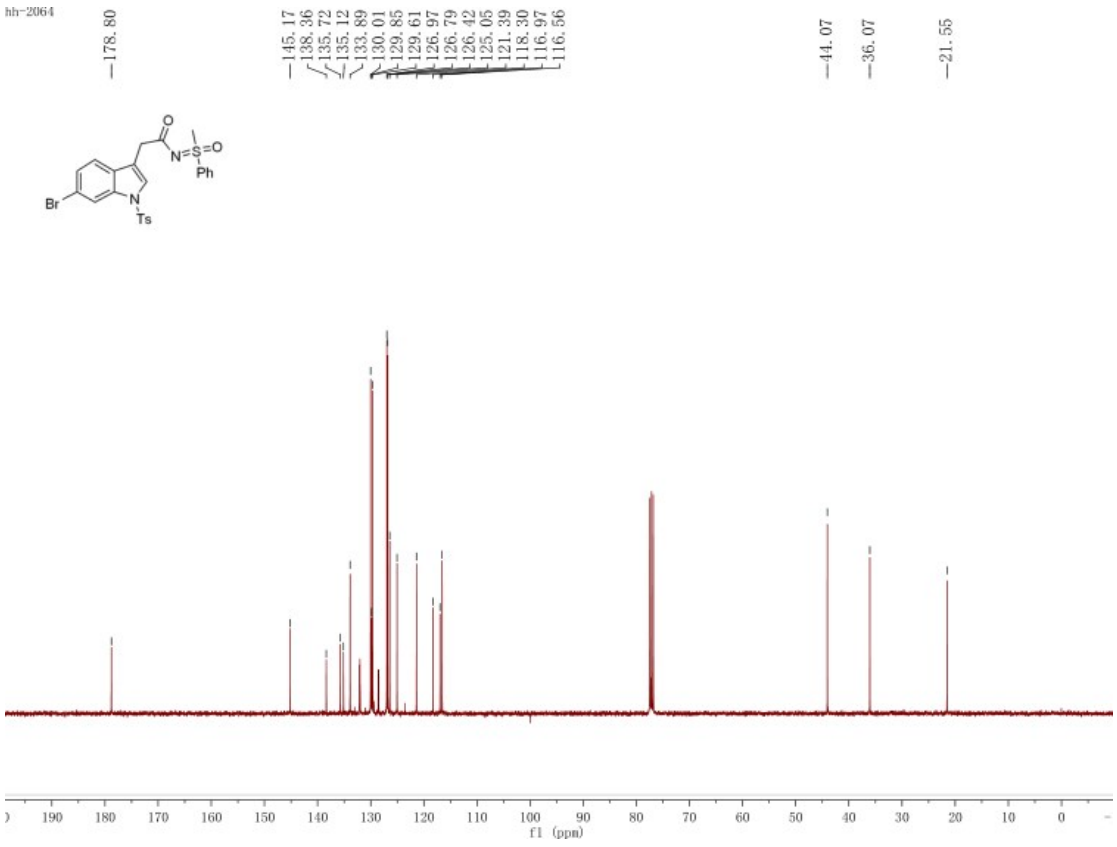
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4i



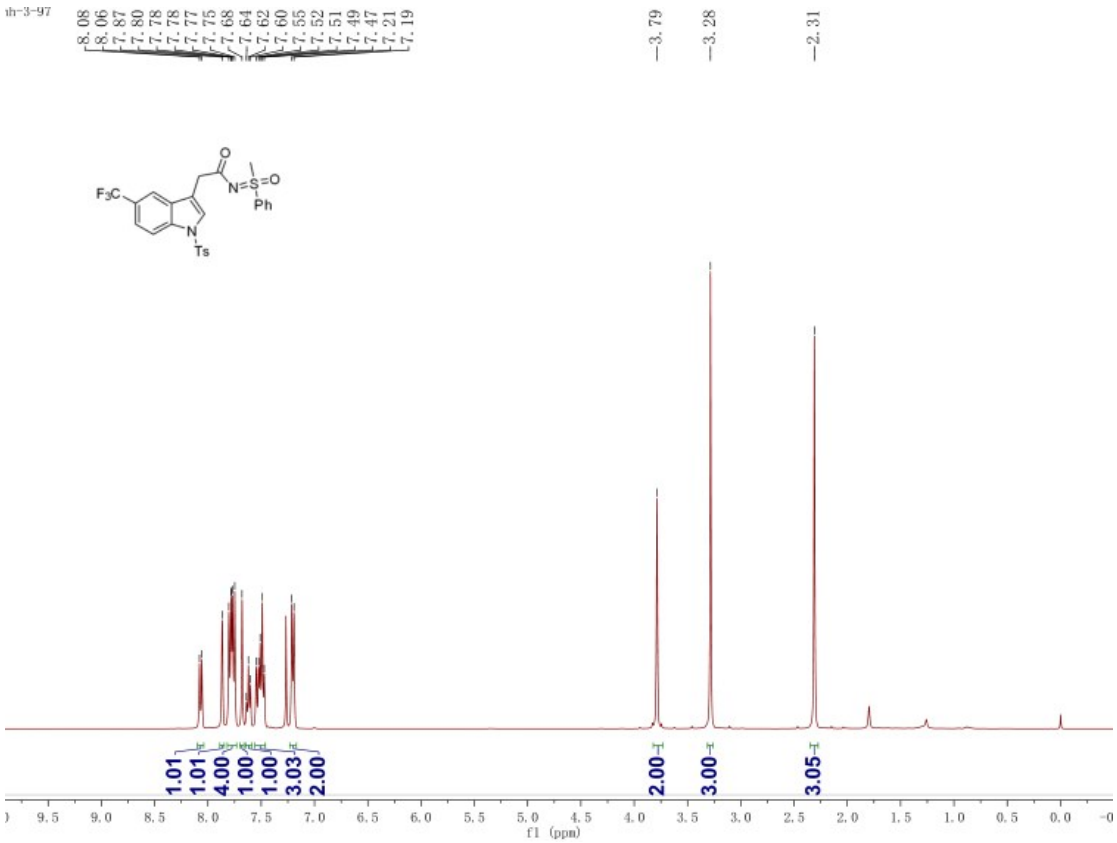
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4j



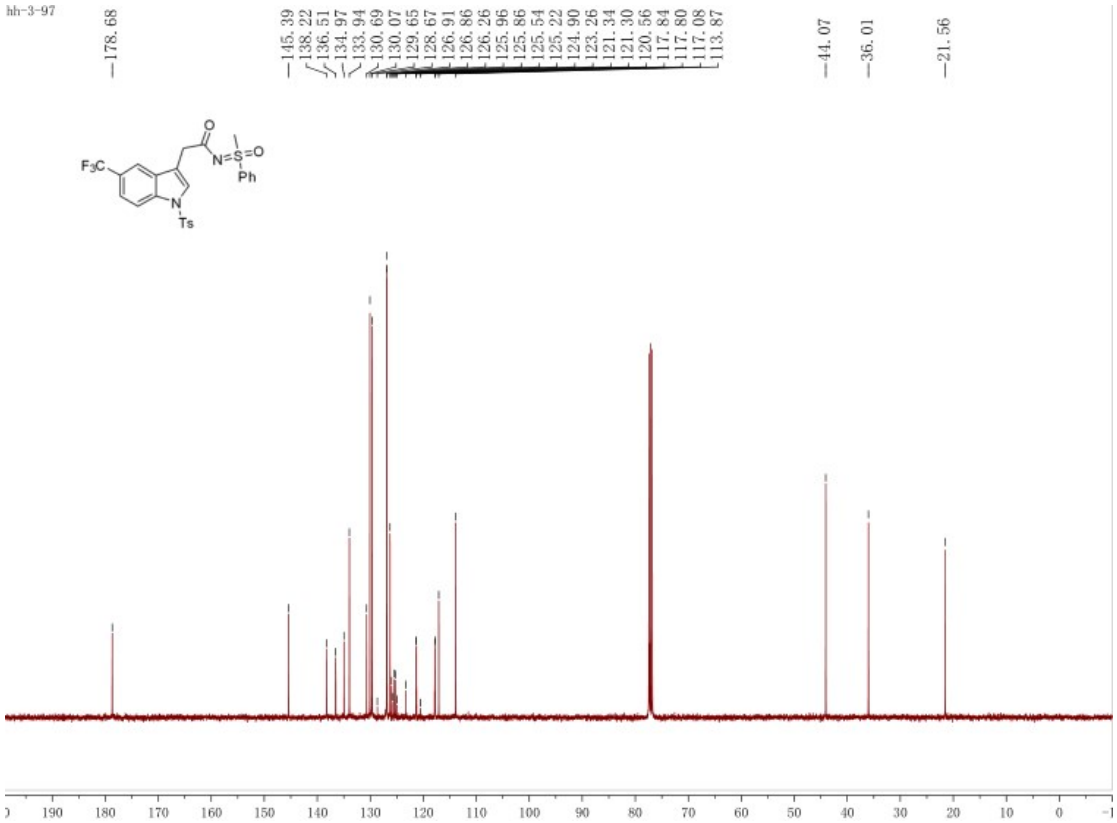
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4j



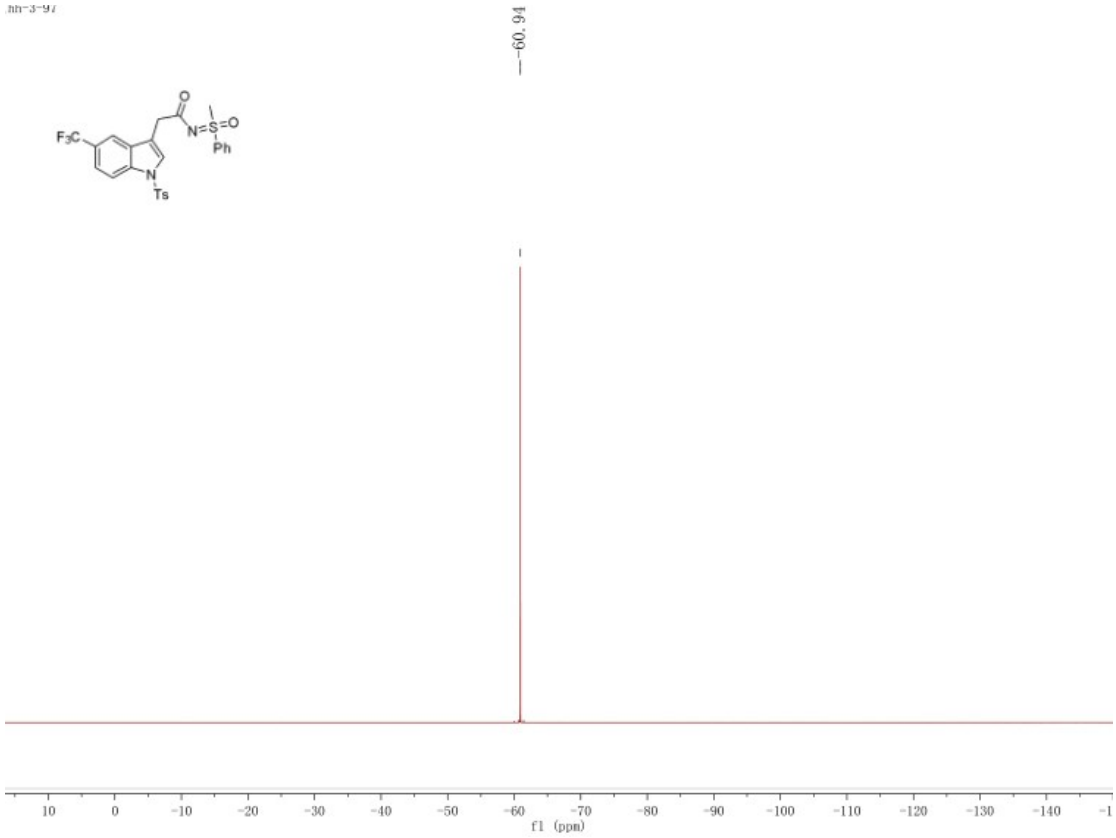
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4k



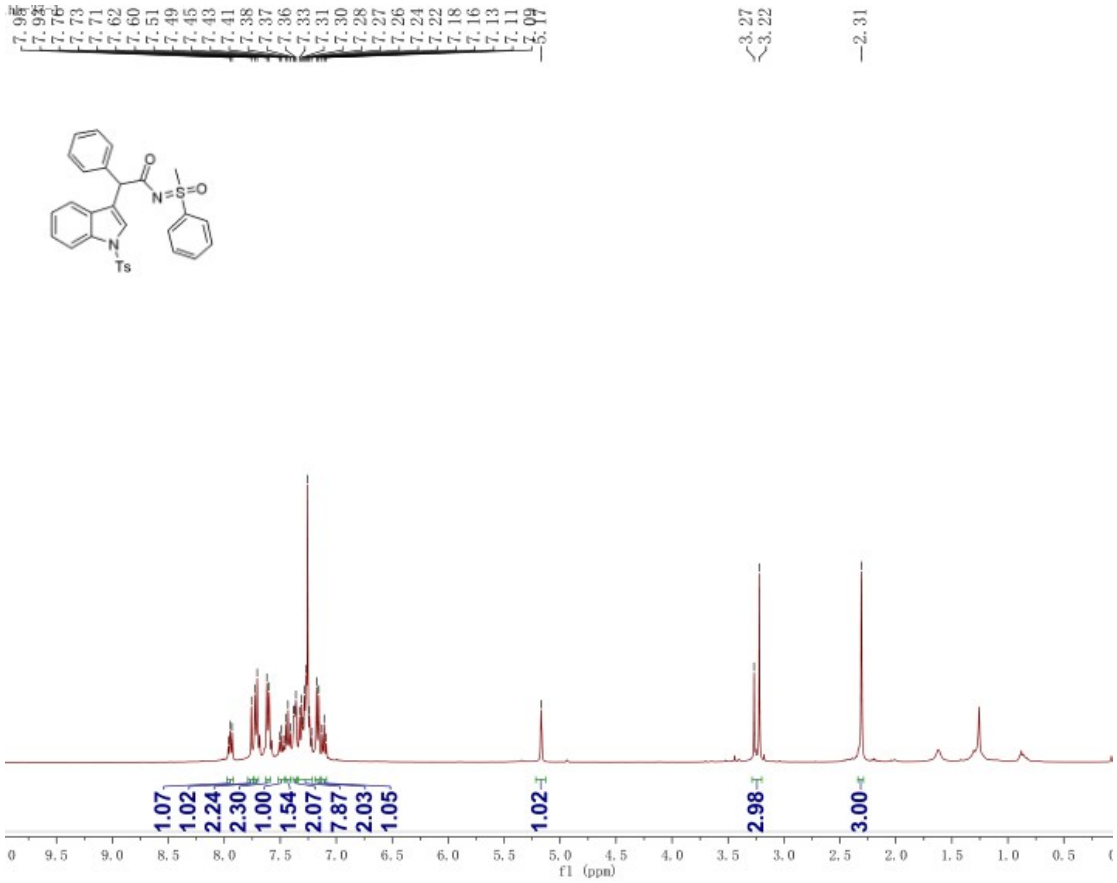
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4k



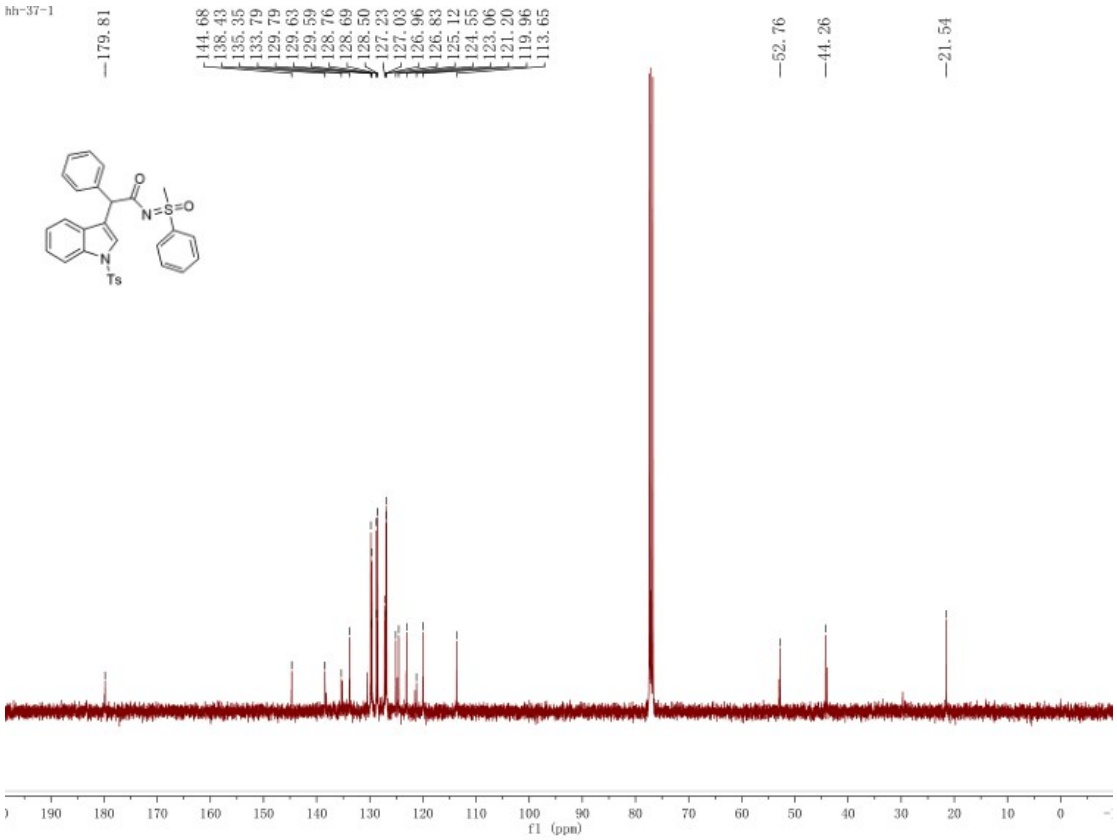
^{19}F NMR (376 MHz, $CDCl_3$) of 4k



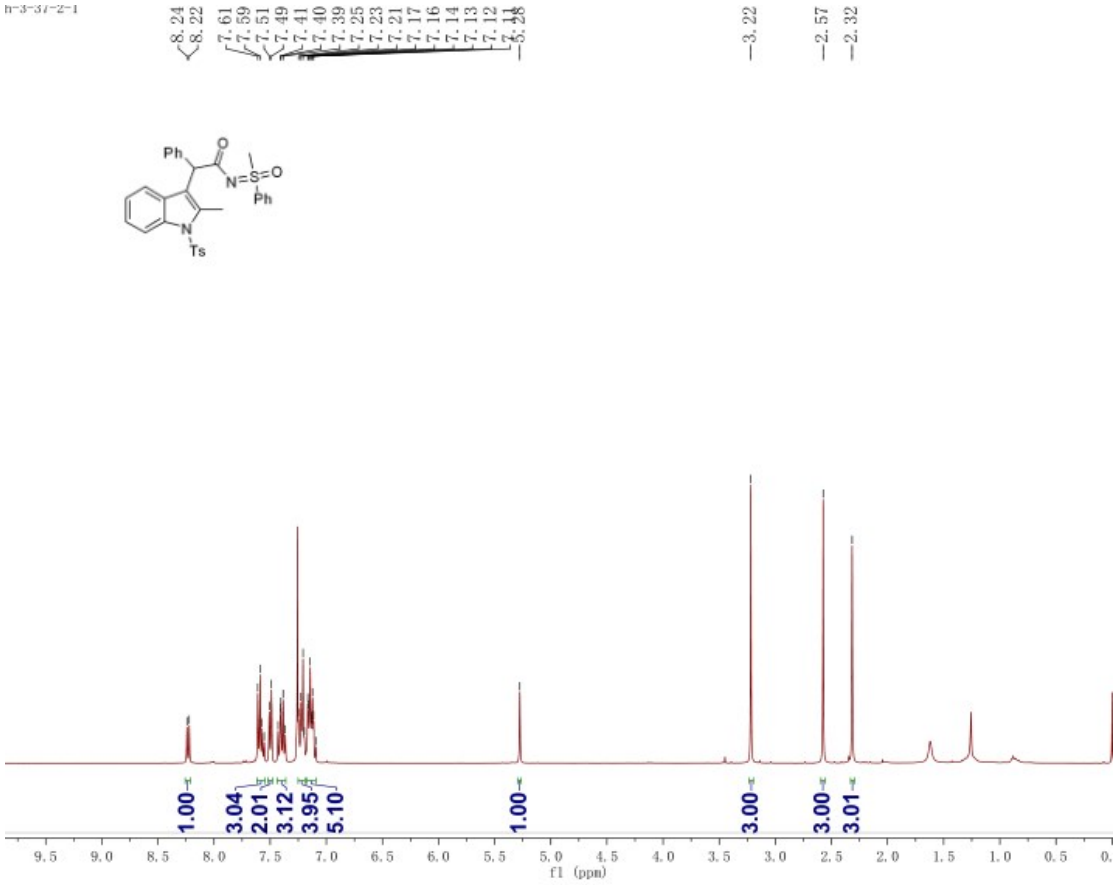
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4l



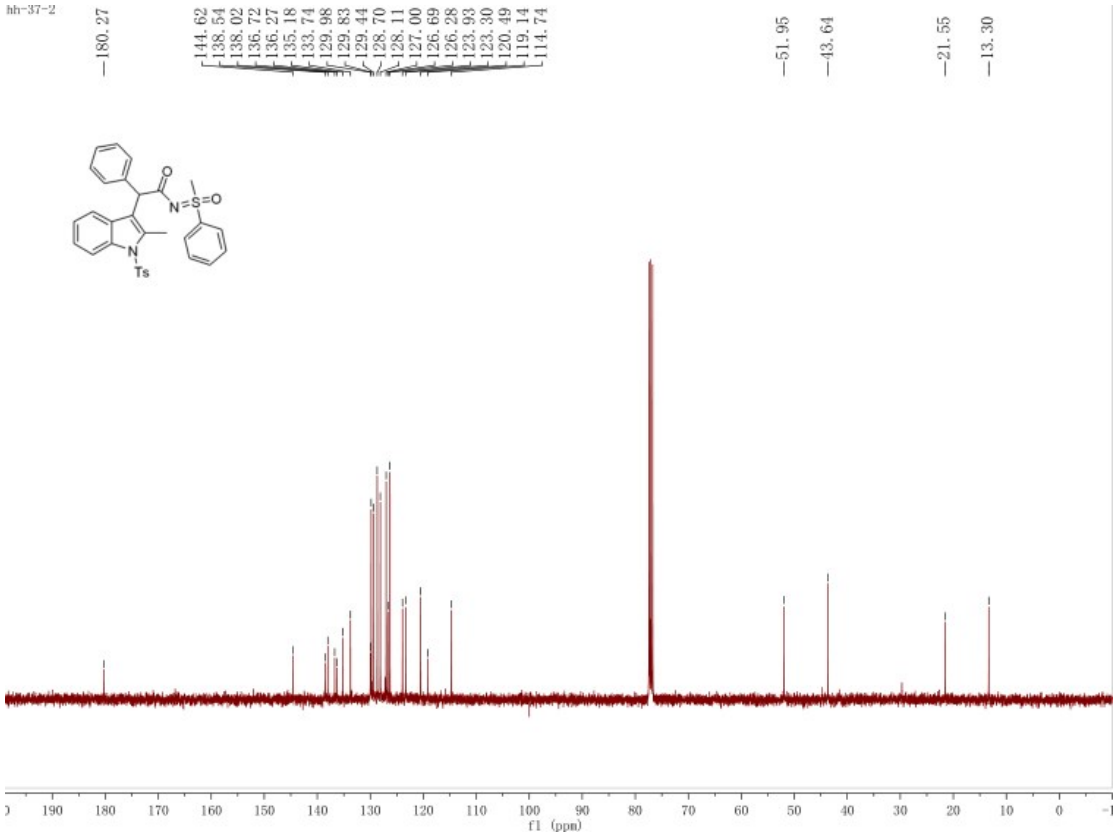
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4l



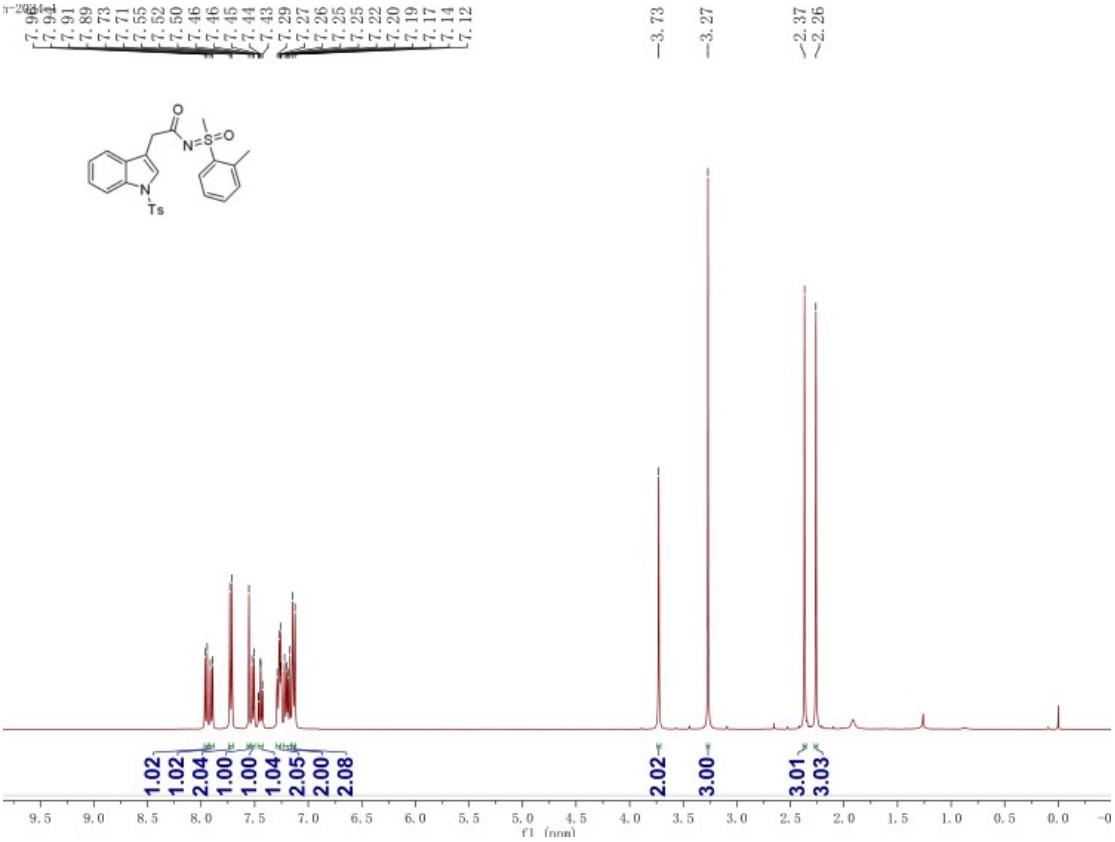
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4m



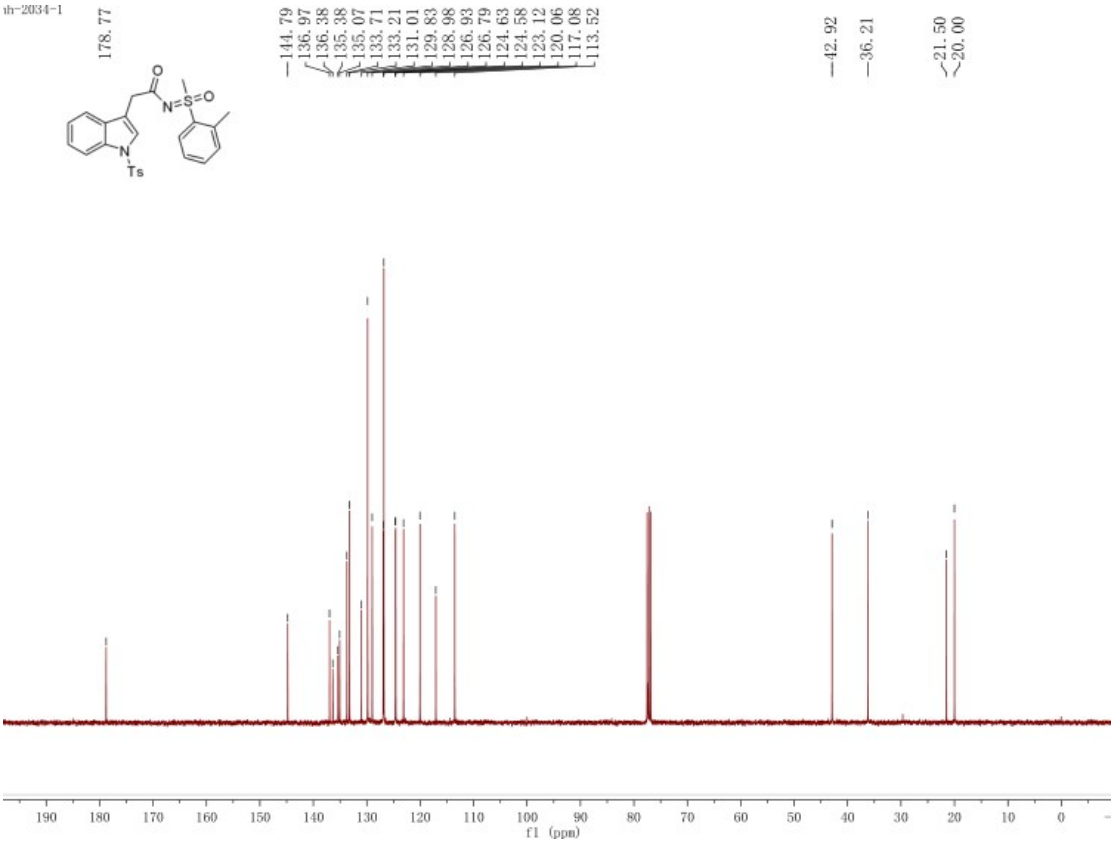
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4m



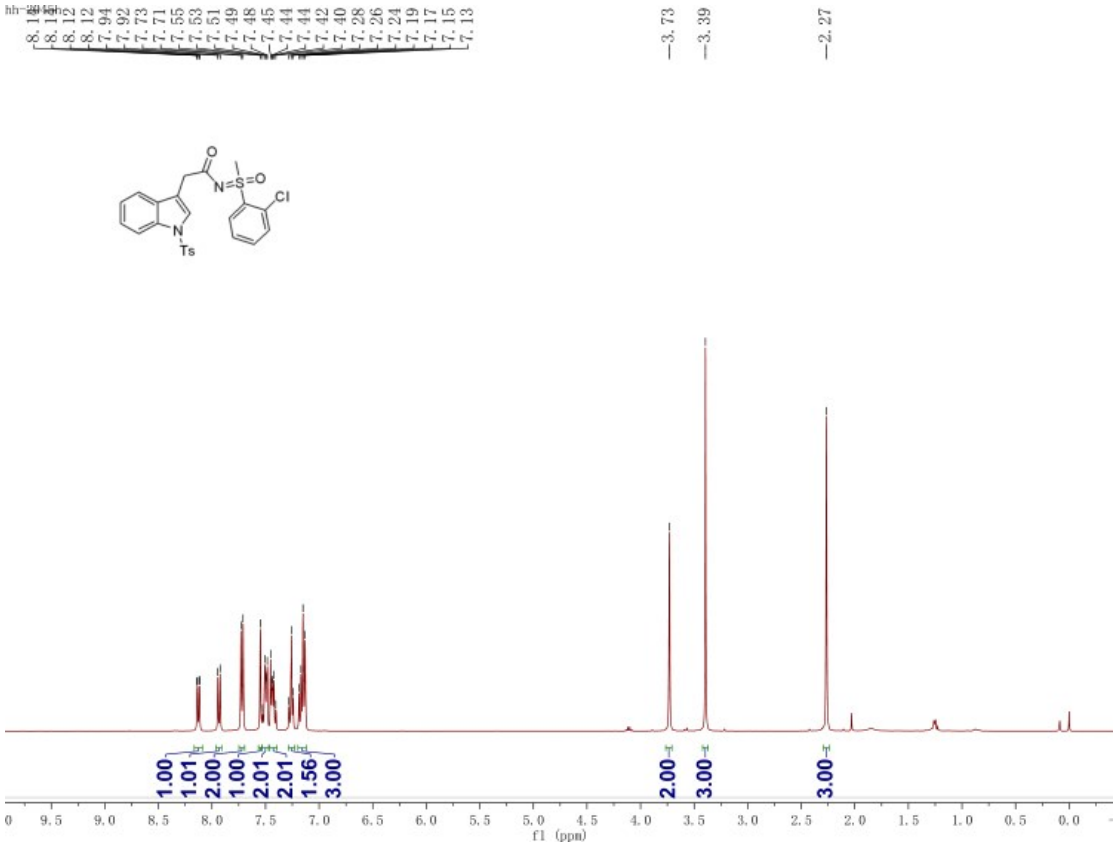
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4n



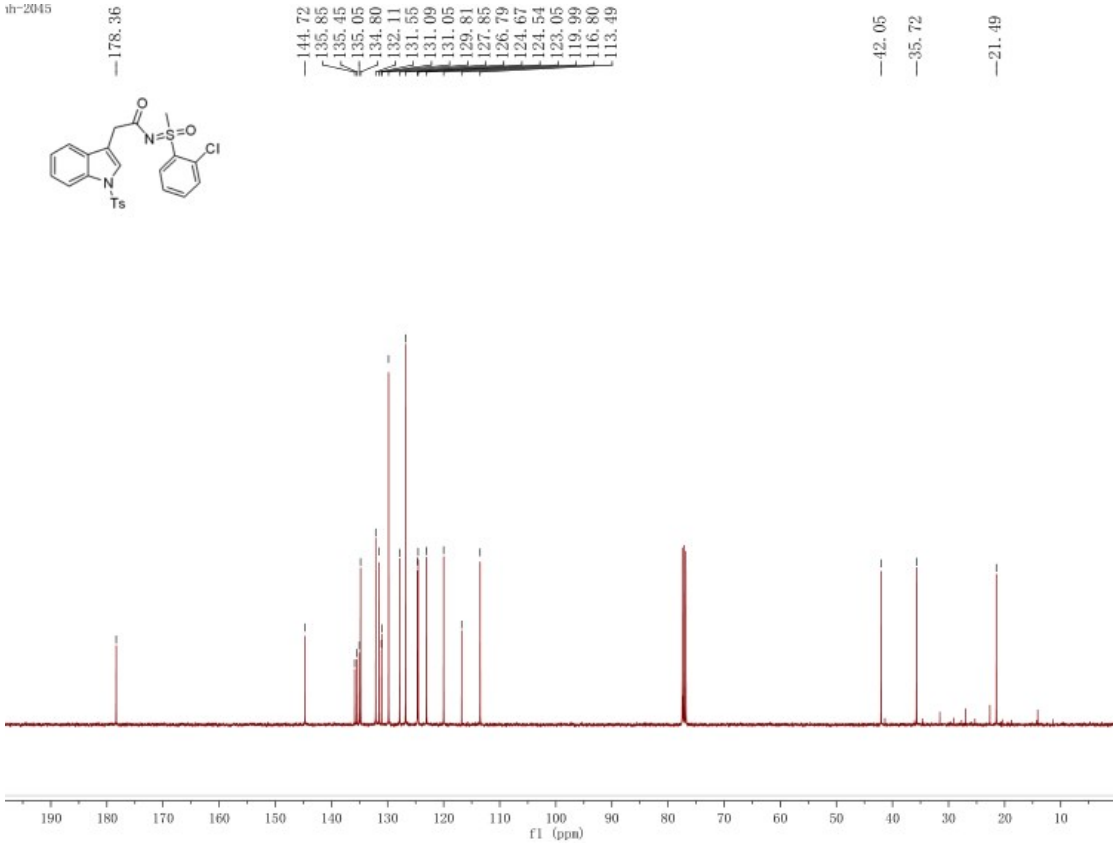
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4n



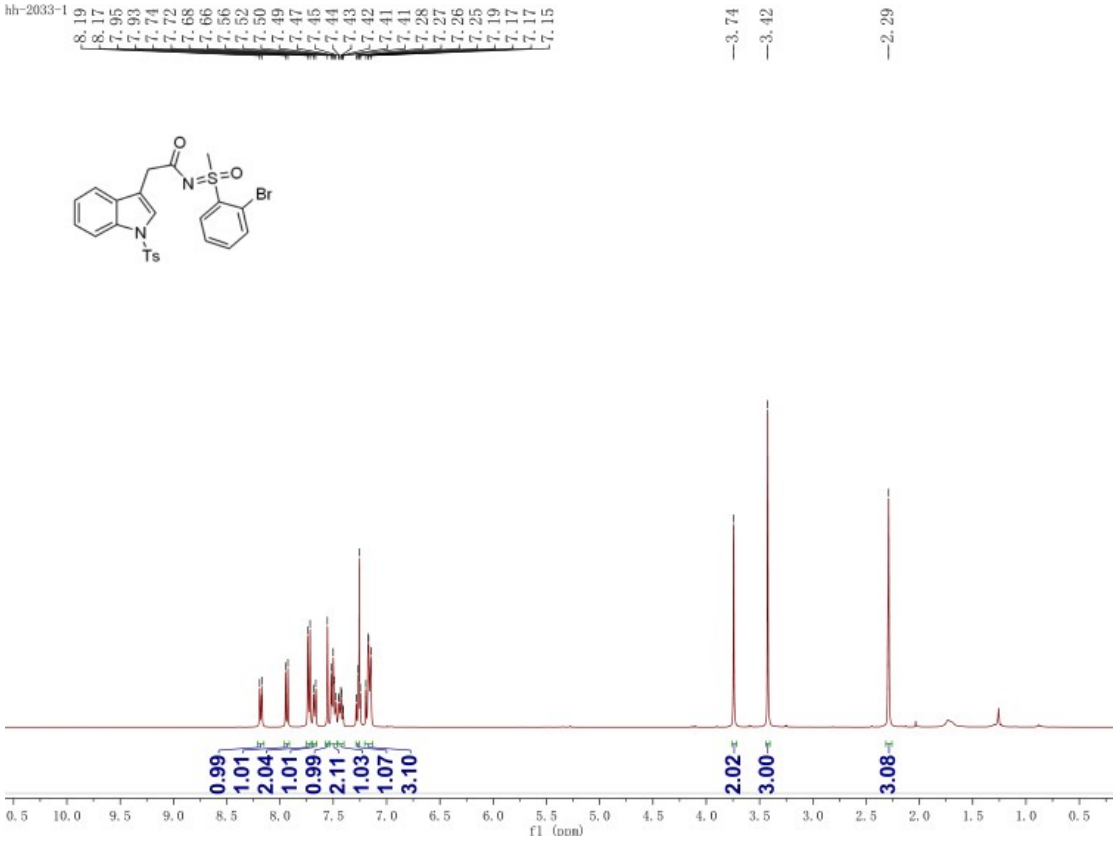
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4o



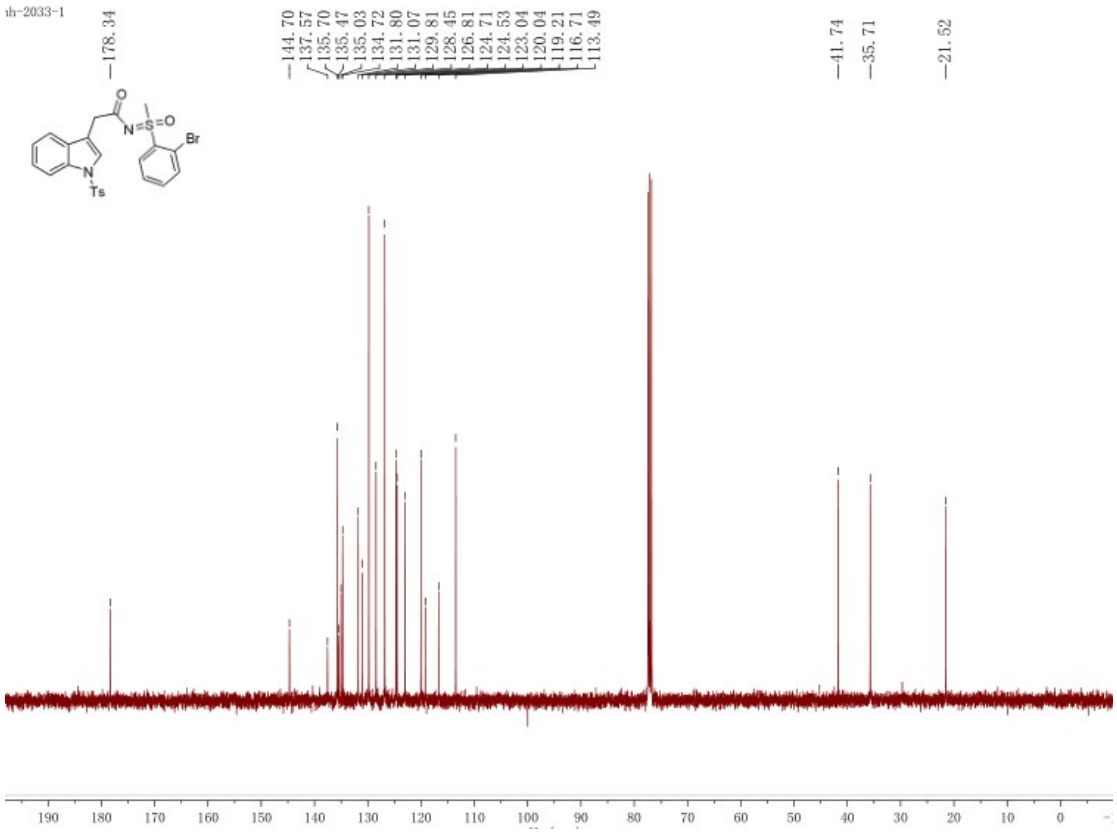
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4o



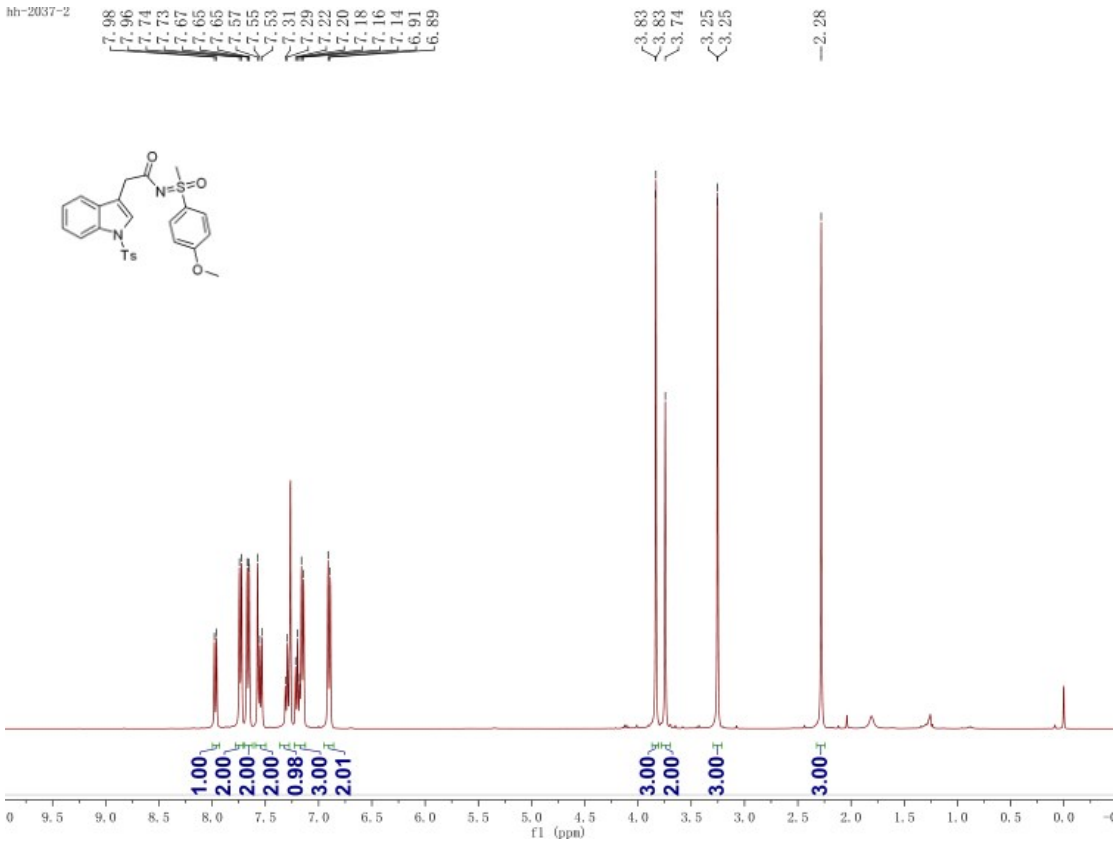
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4p



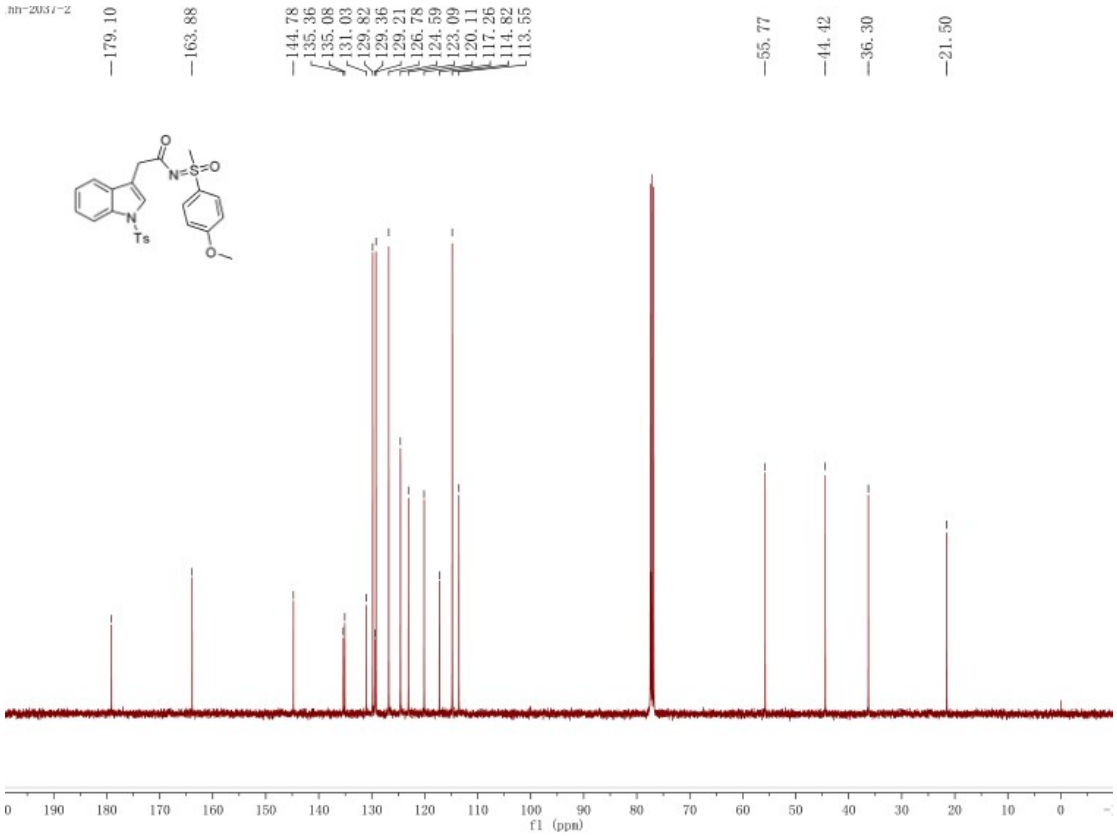
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4p



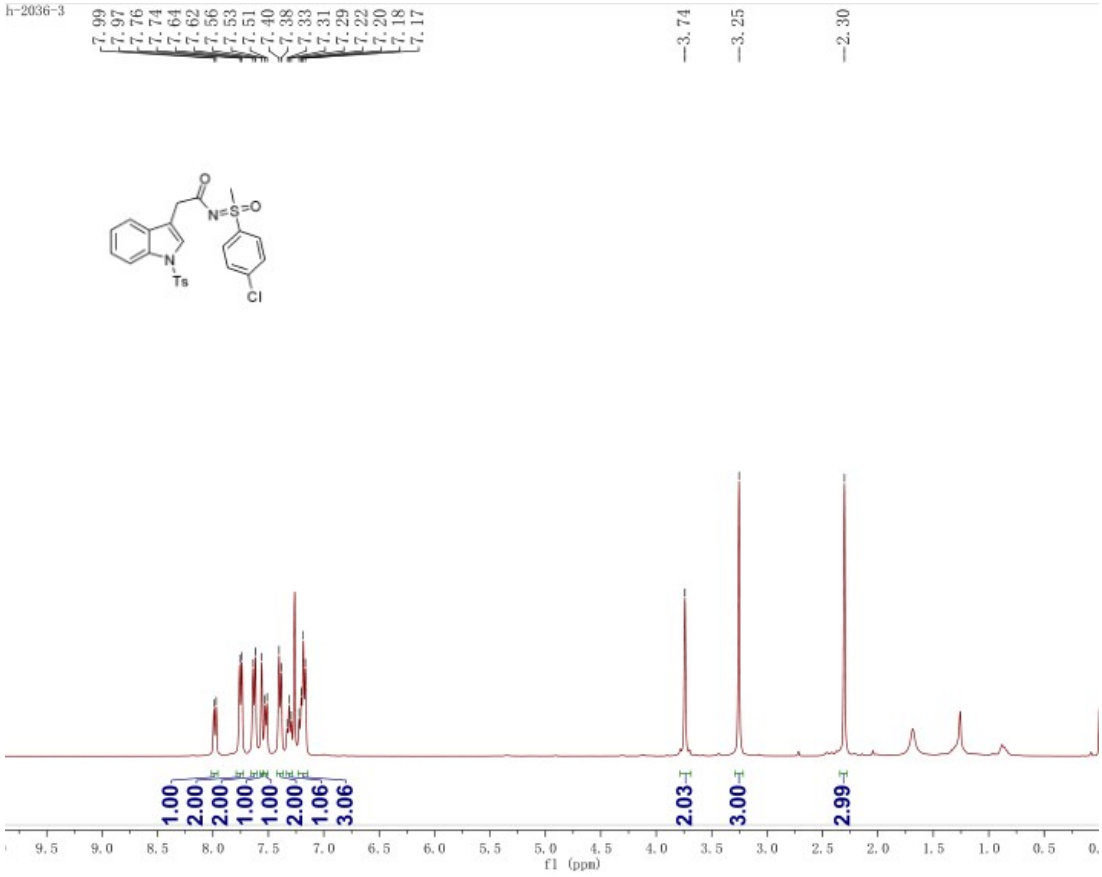
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4q



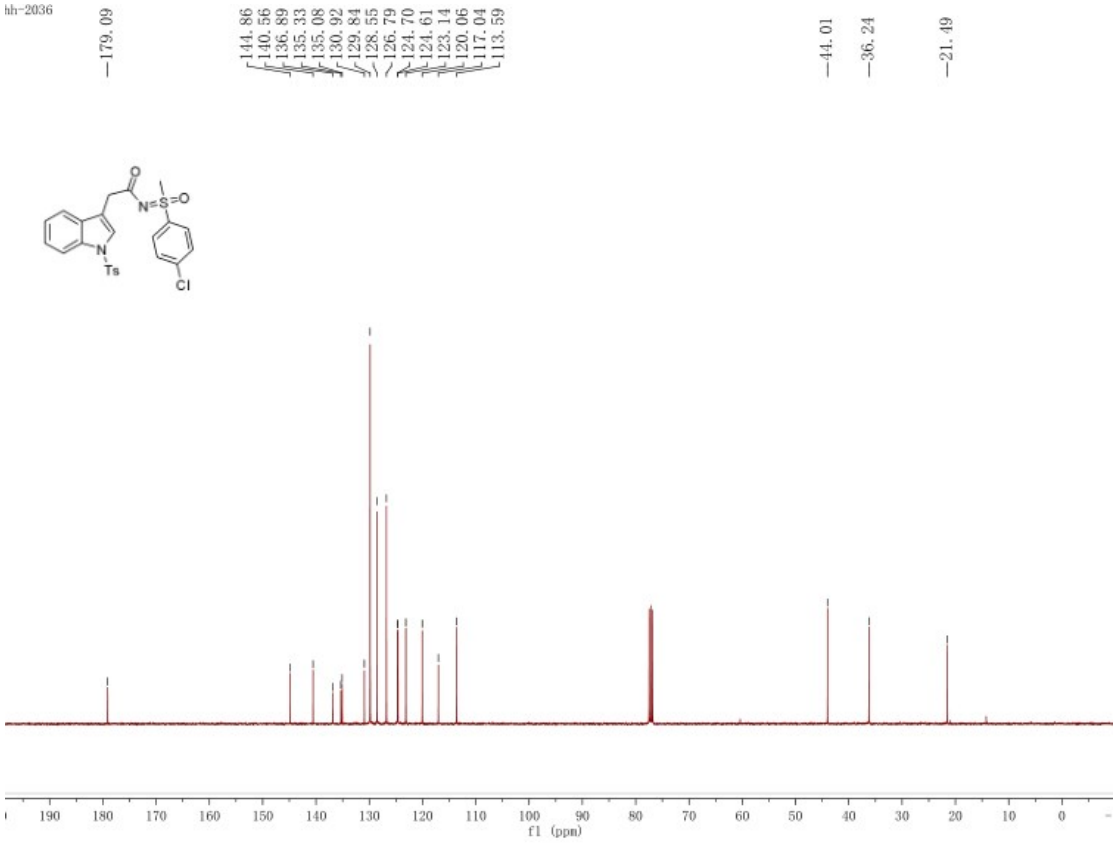
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4q



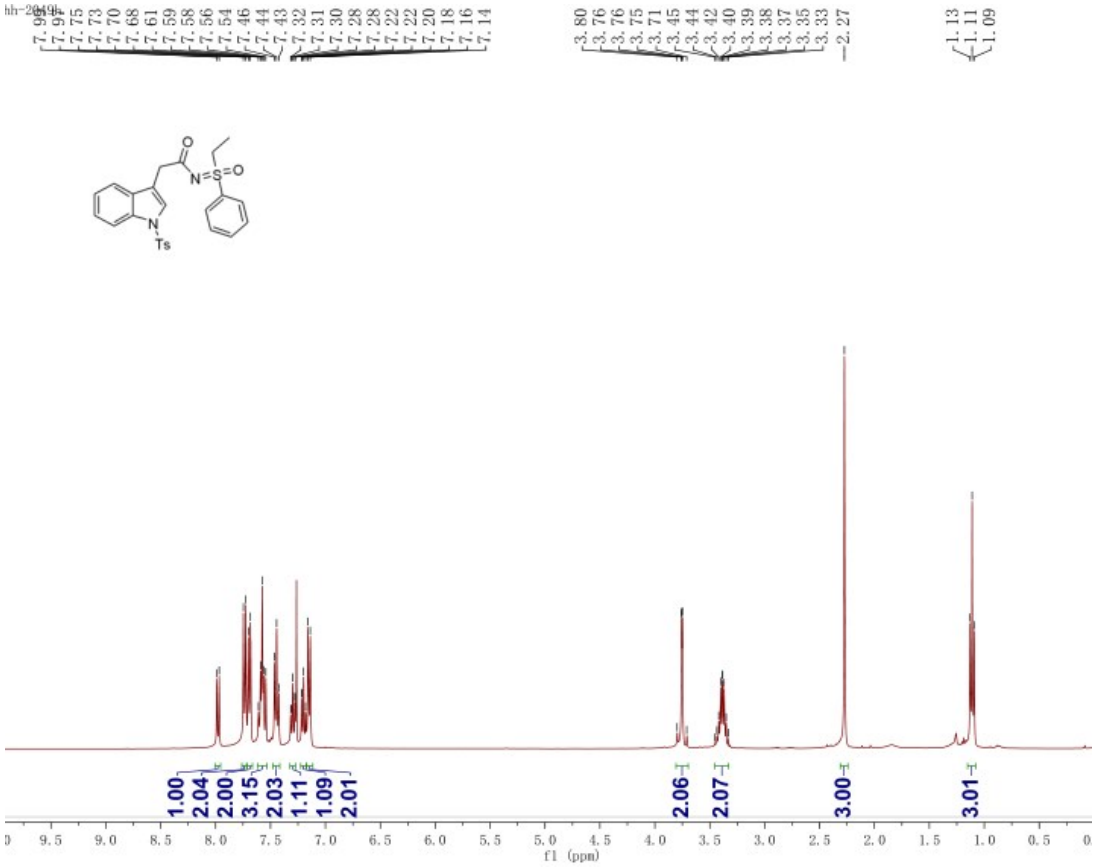
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4r



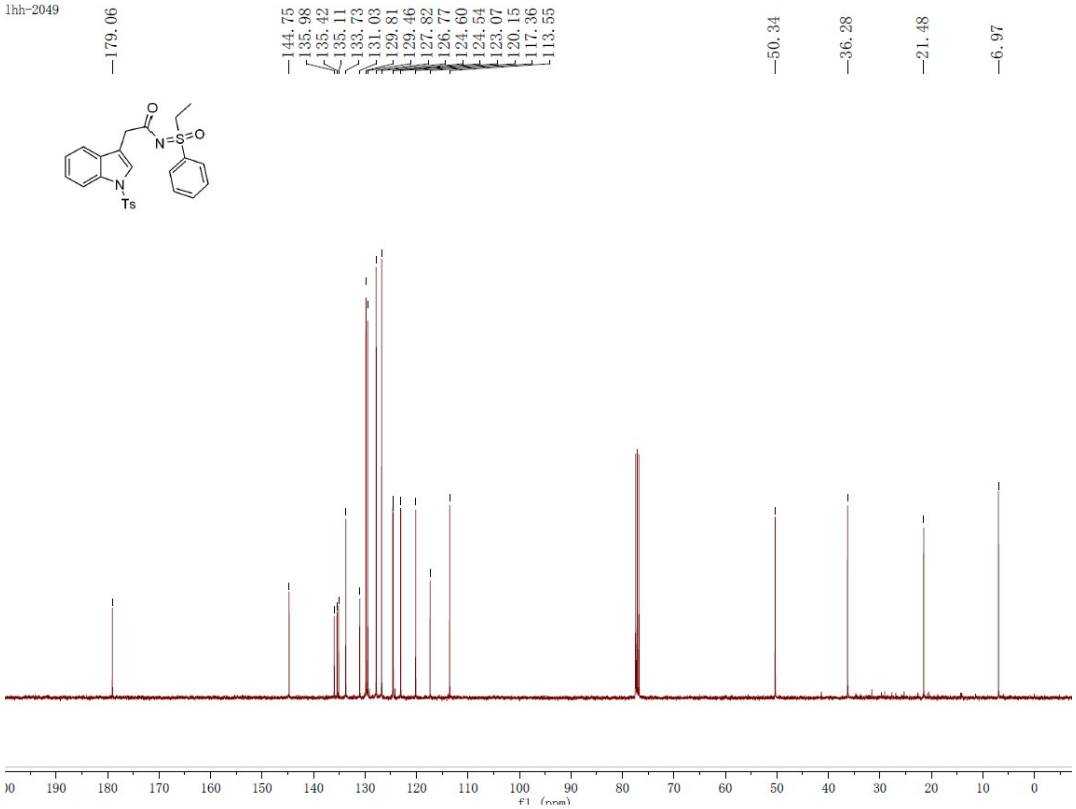
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4r



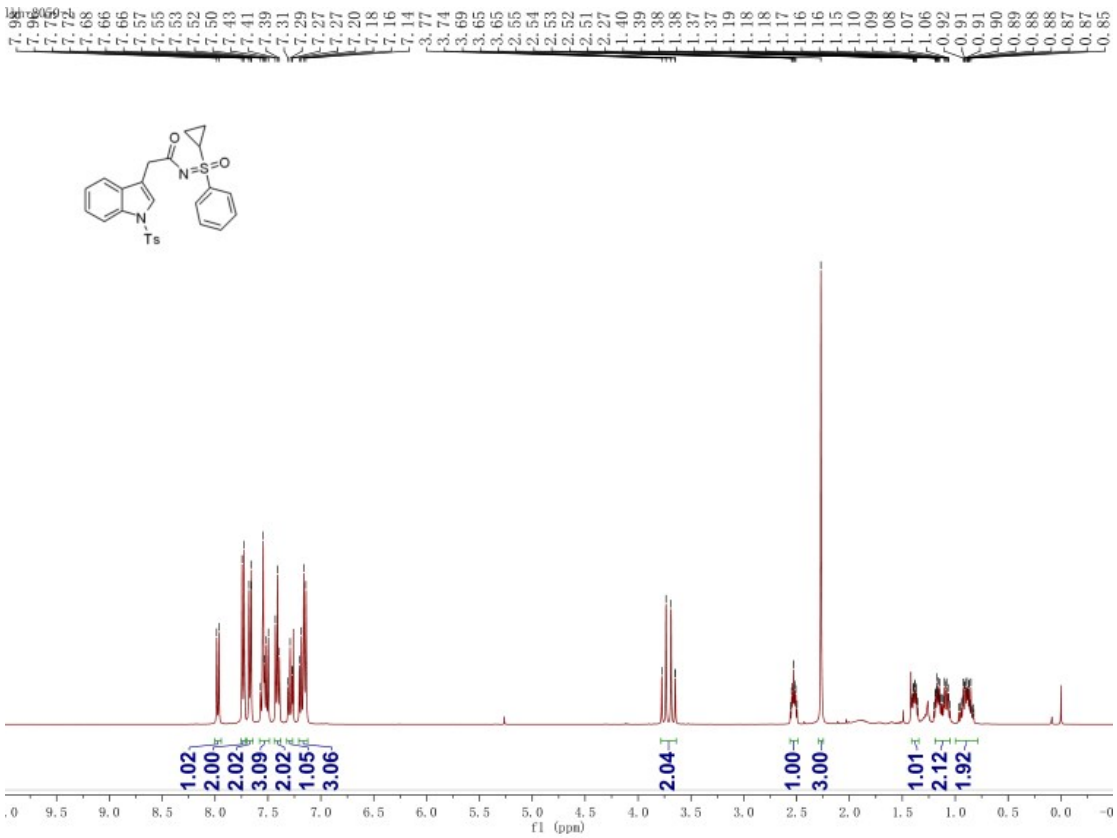
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4s



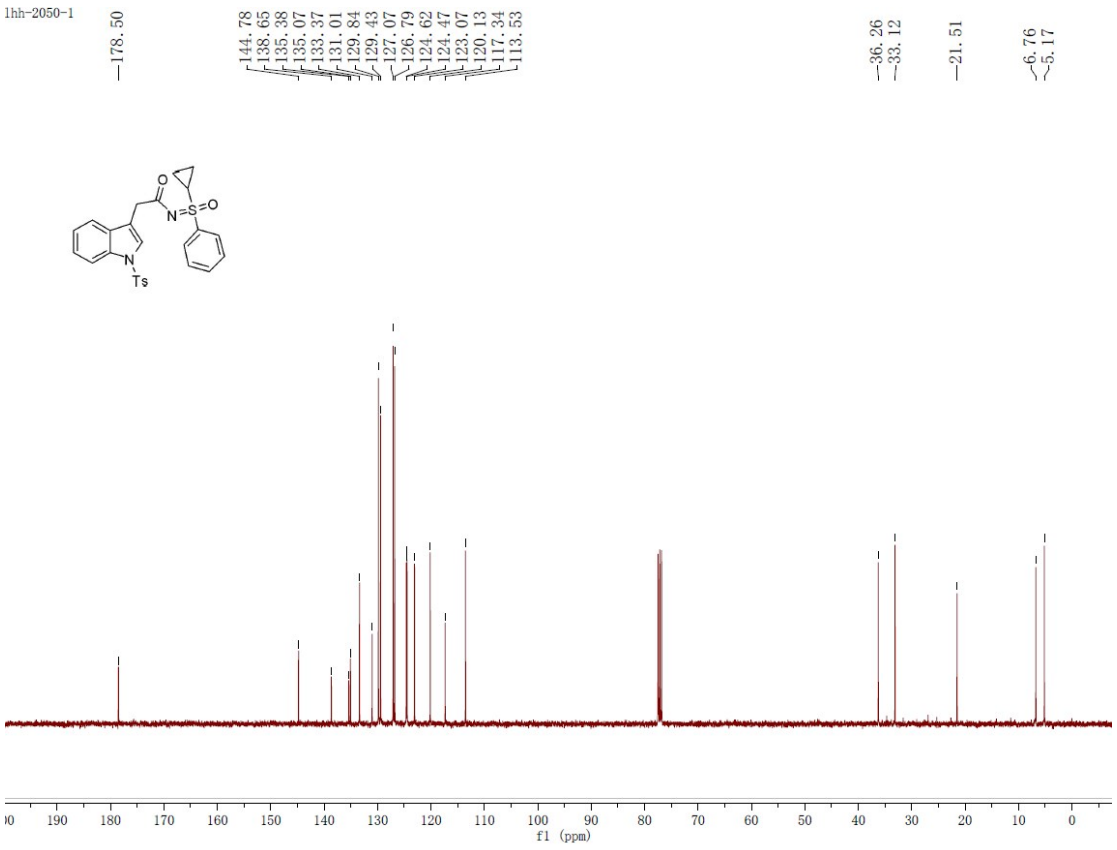
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4s



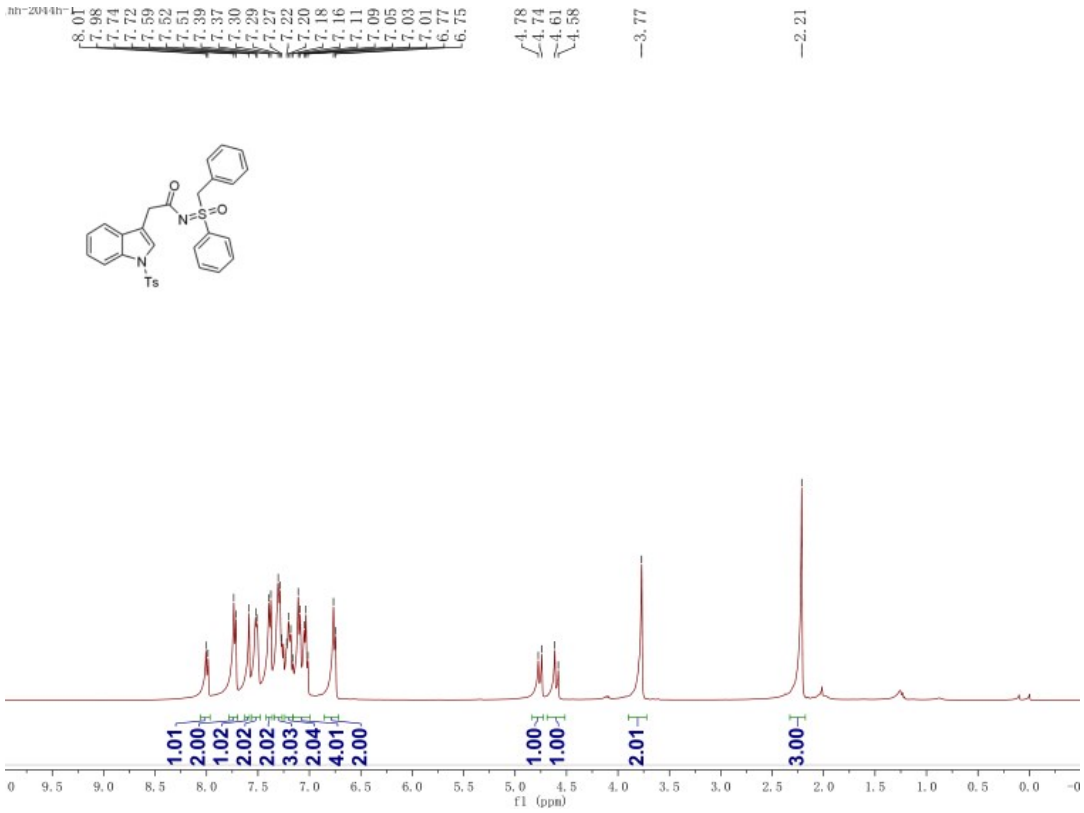
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4t



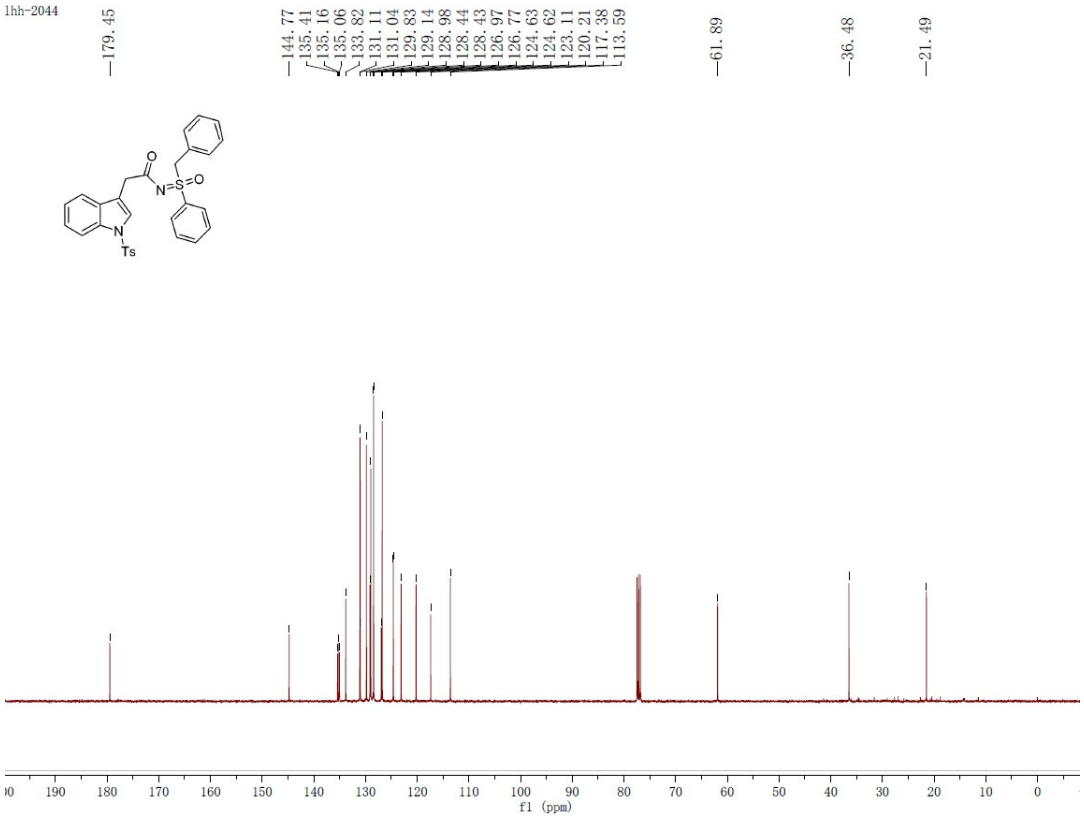
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4t



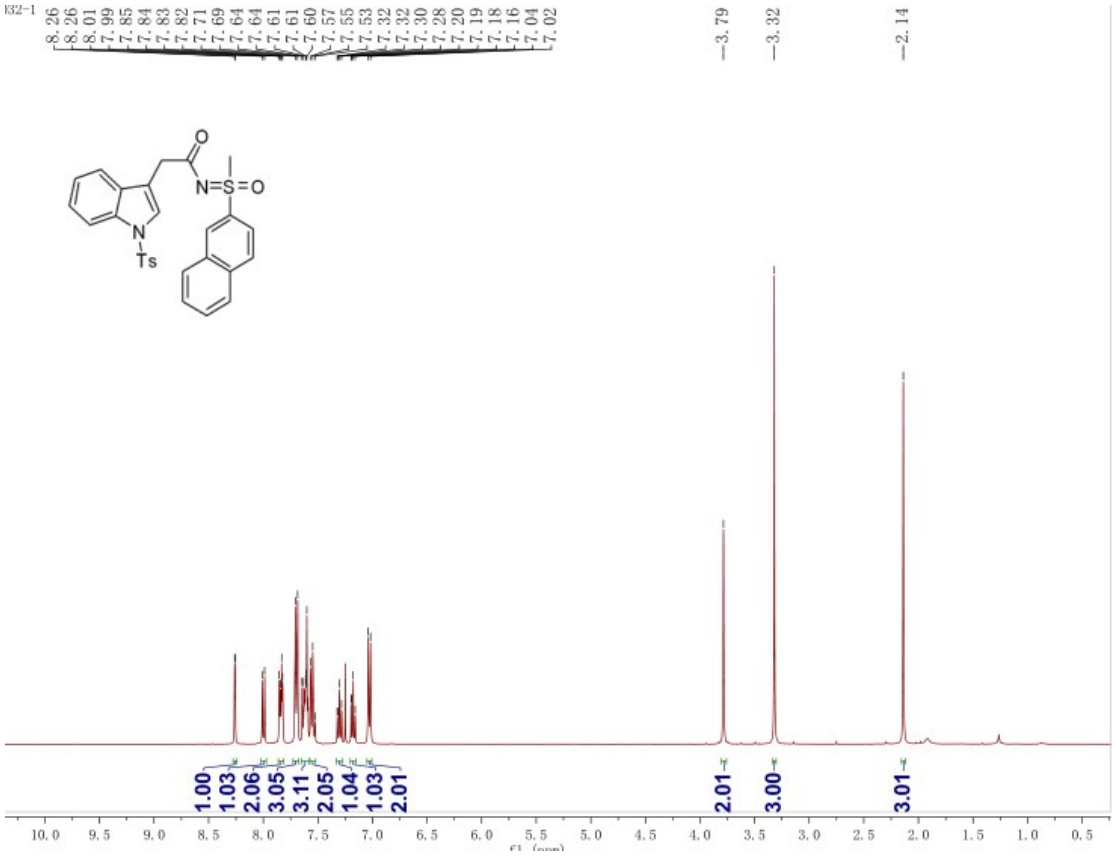
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4u



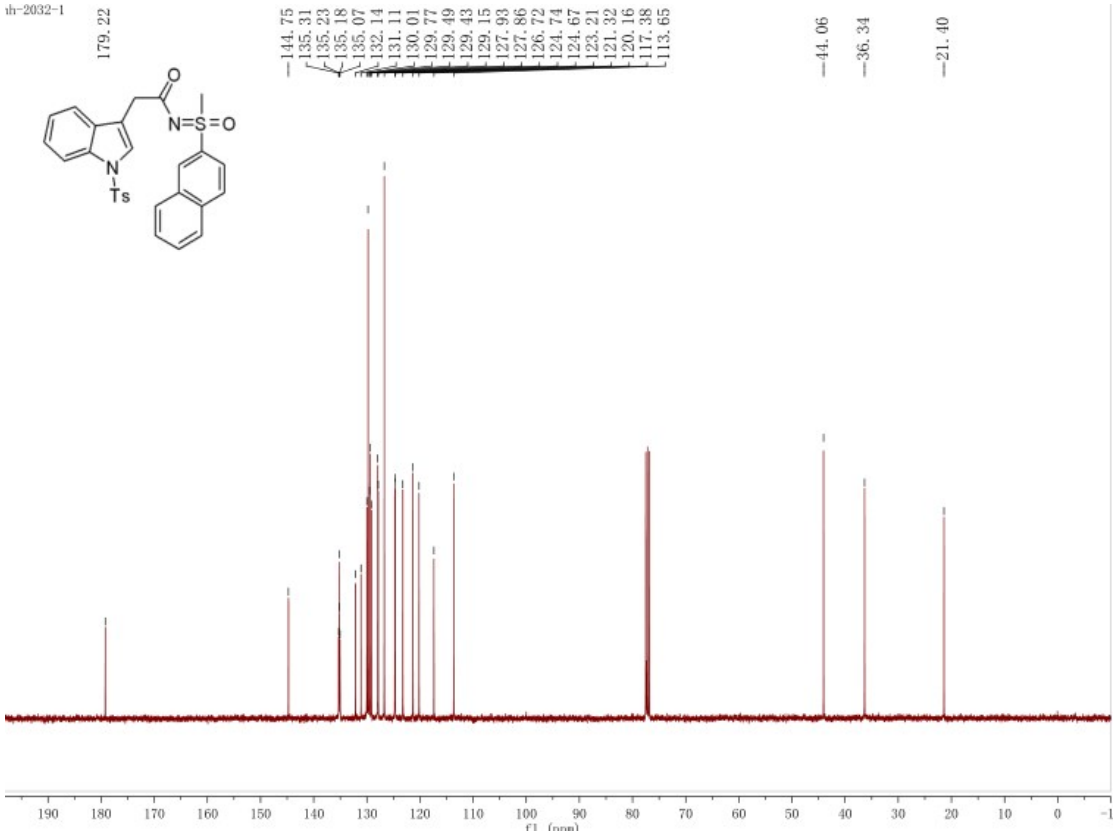
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4u



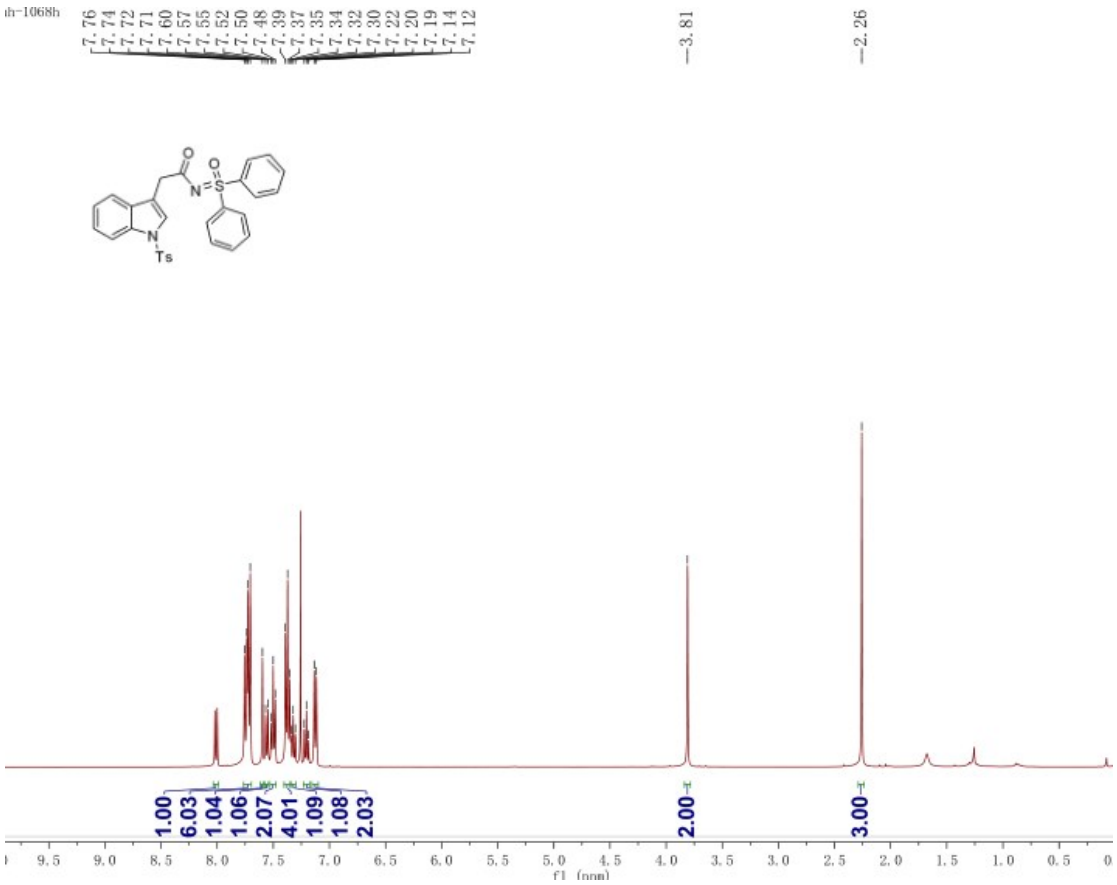
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4v



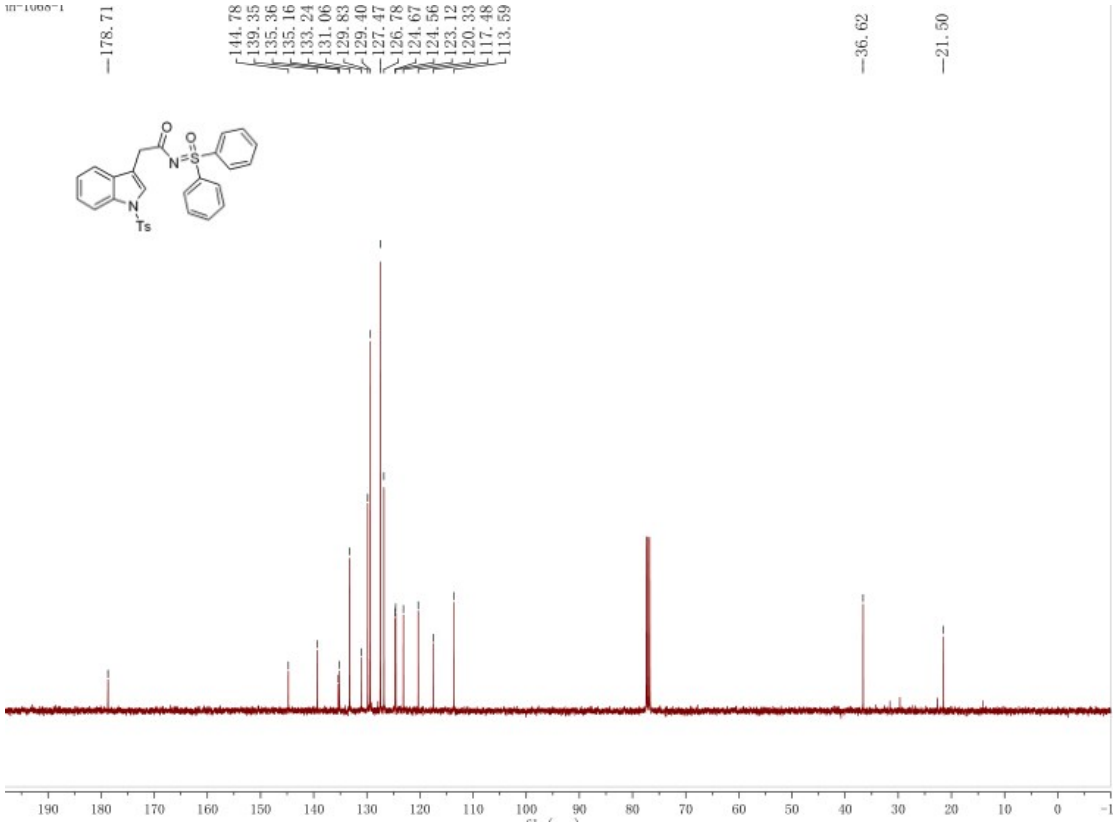
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4v



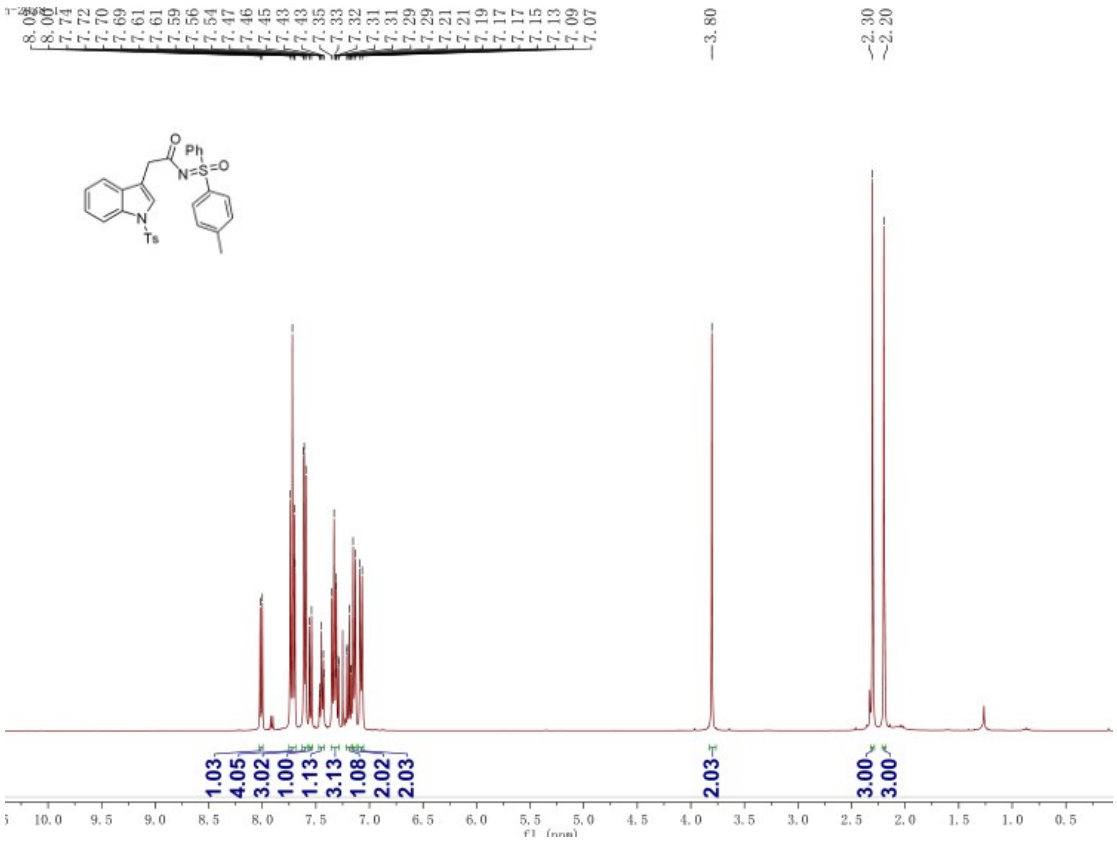
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4w



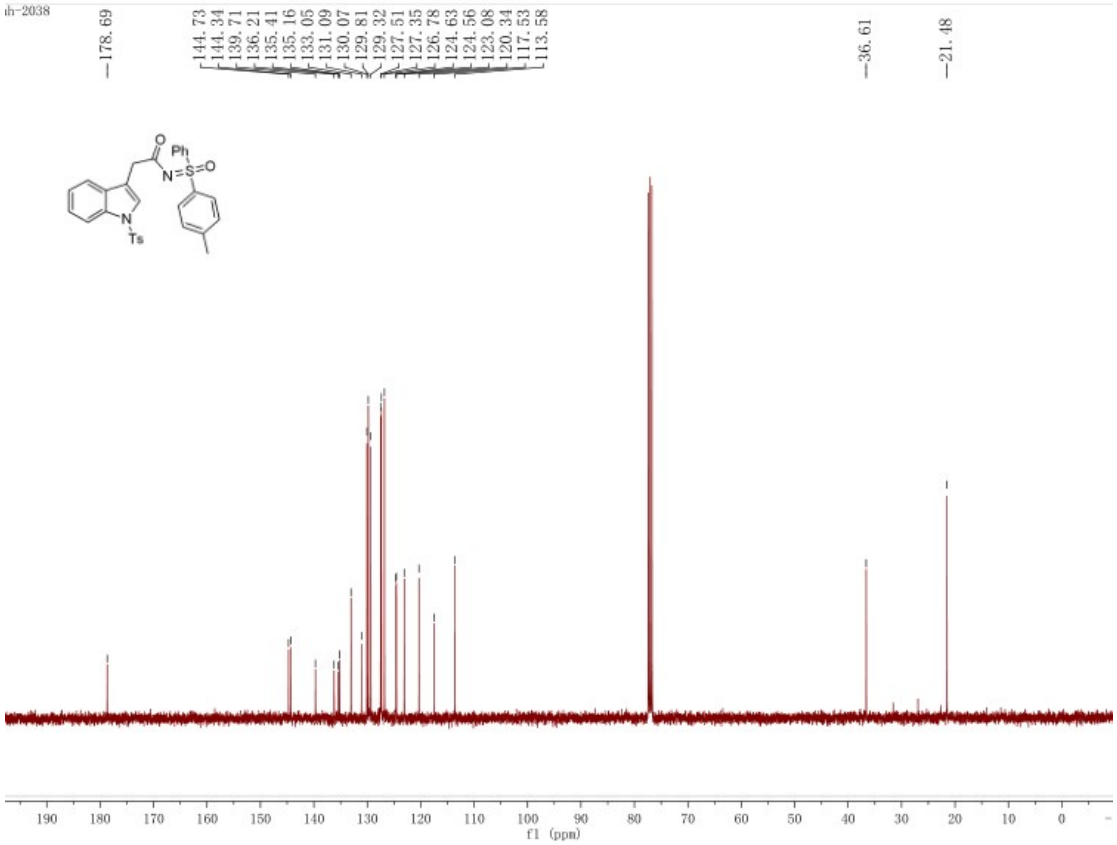
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4w



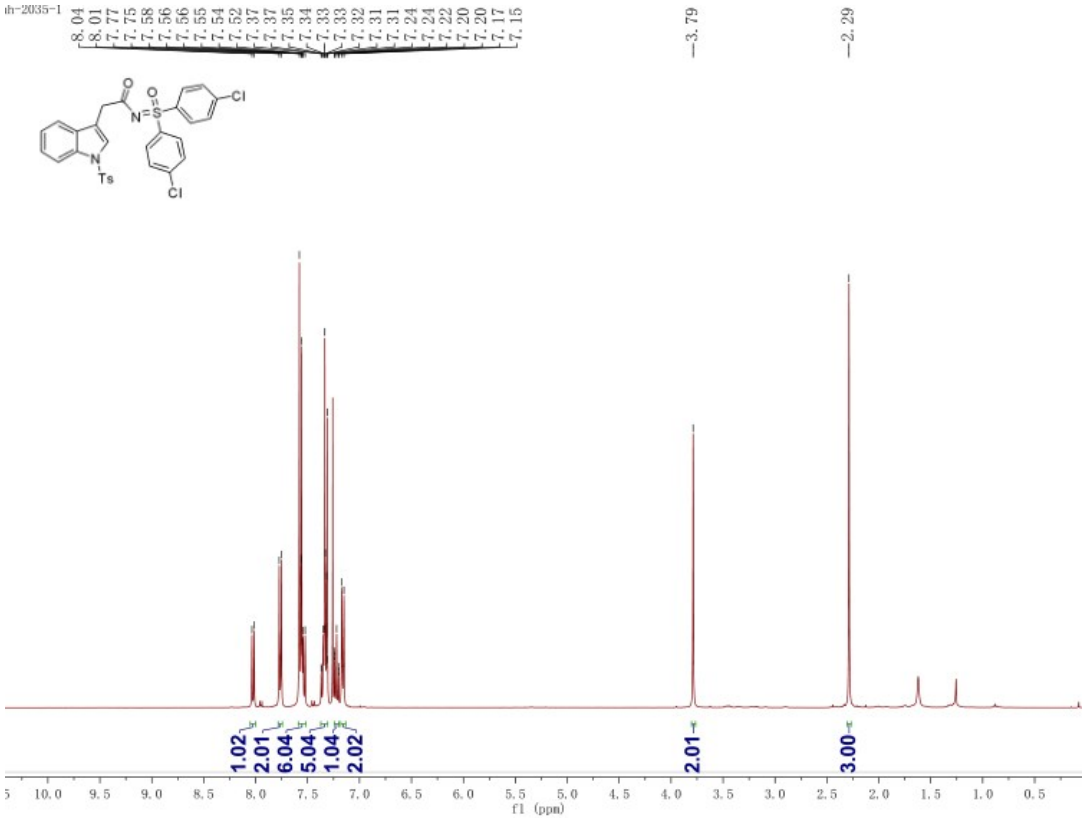
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4x



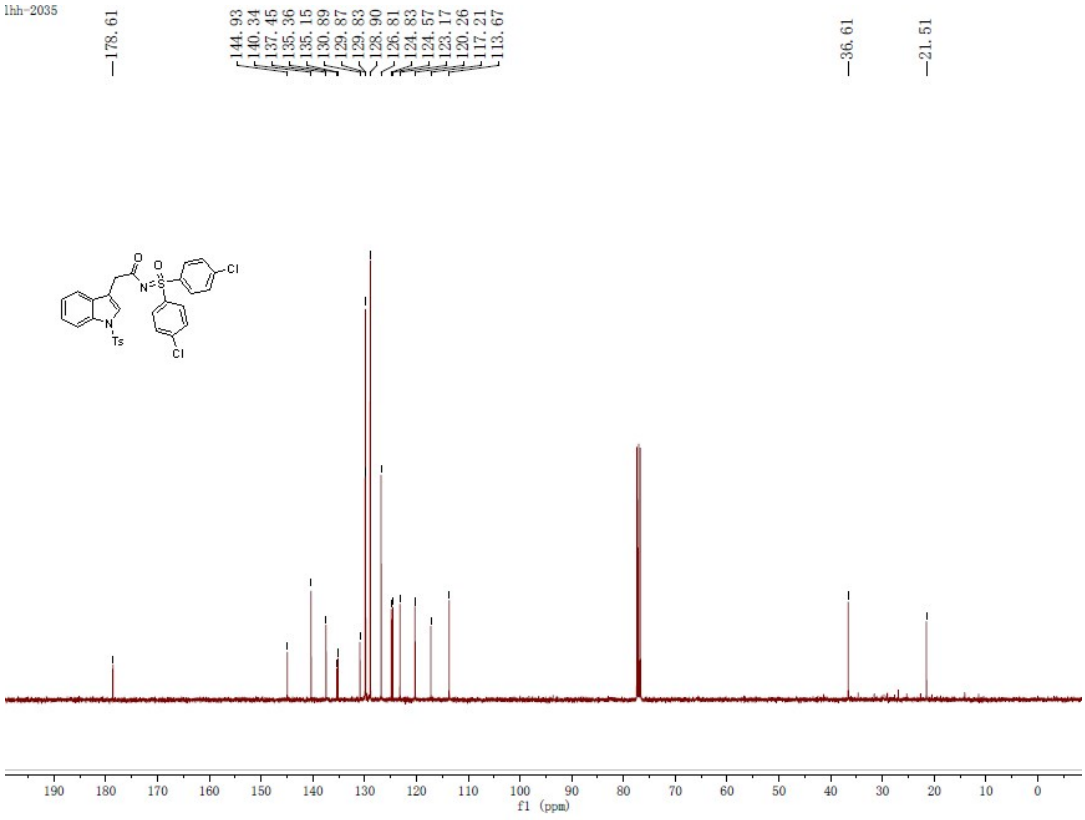
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4x



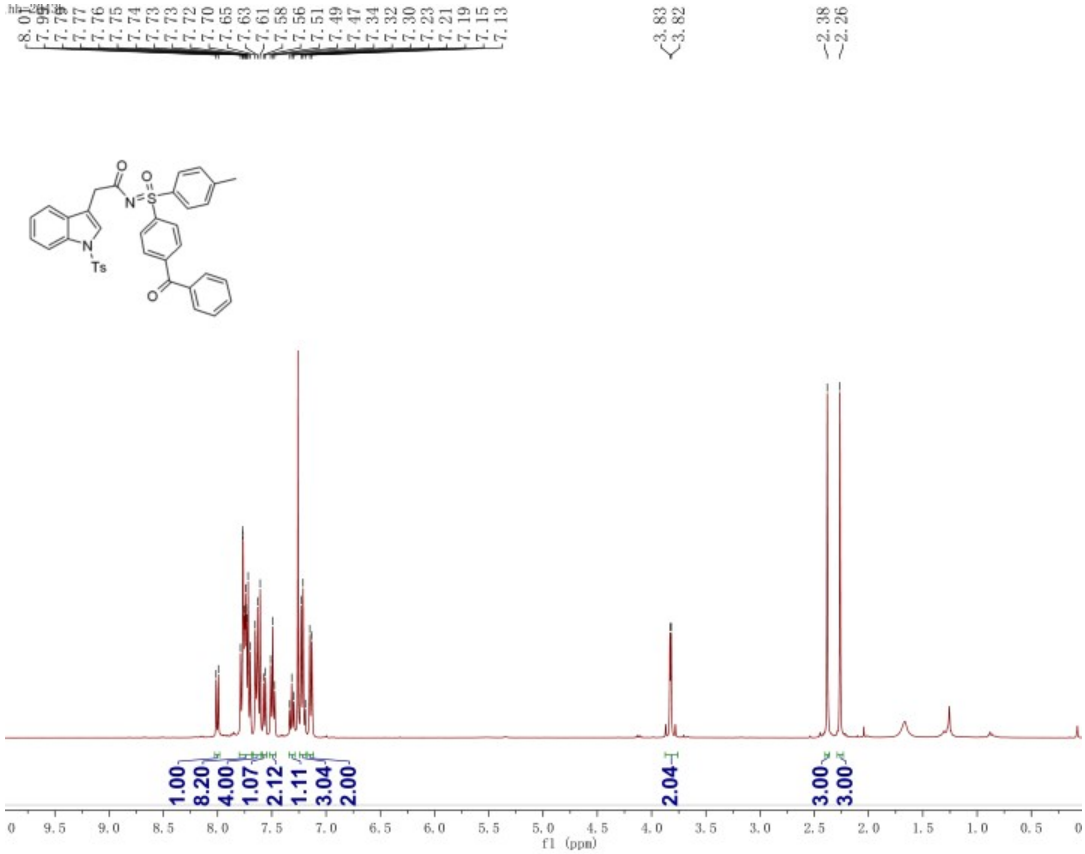
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4y



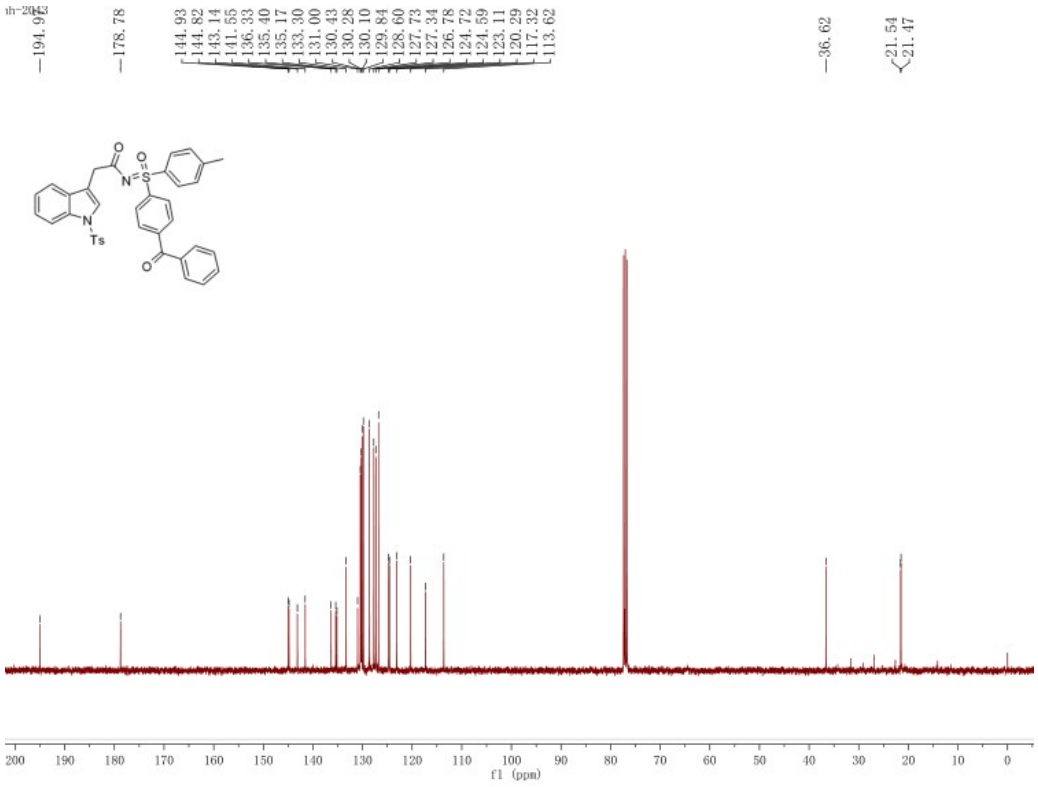
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4y



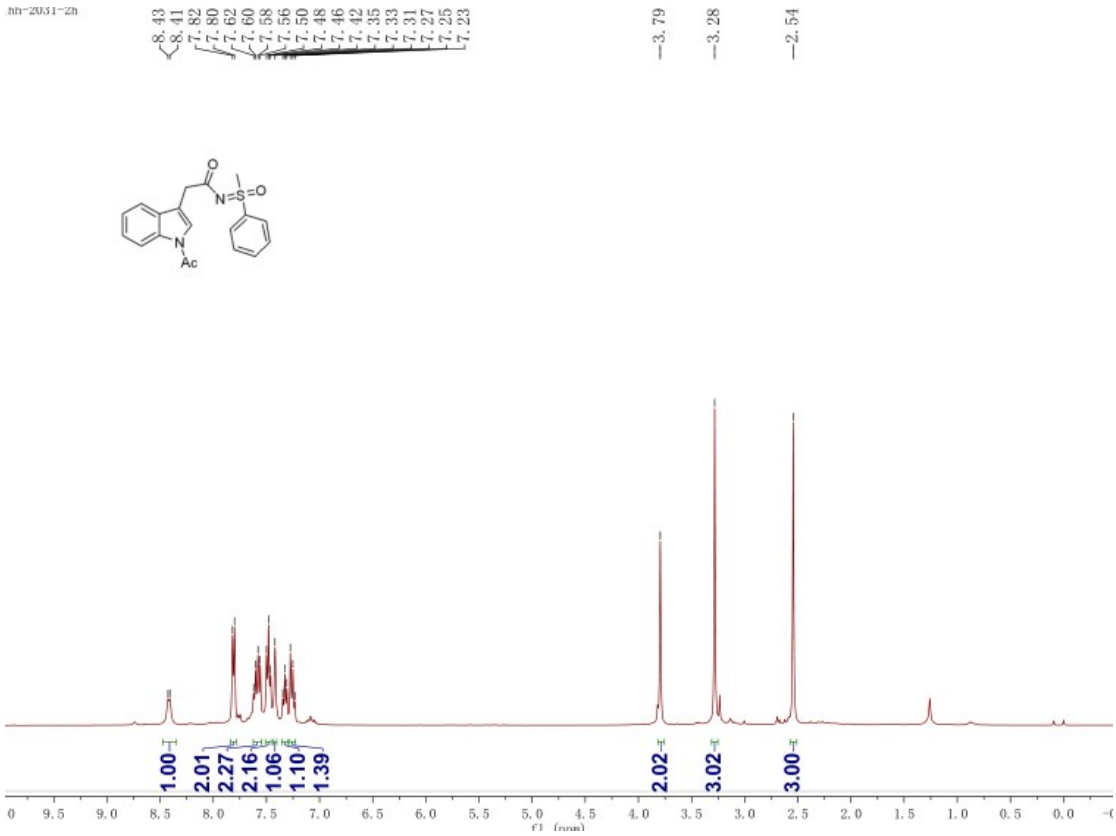
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4z



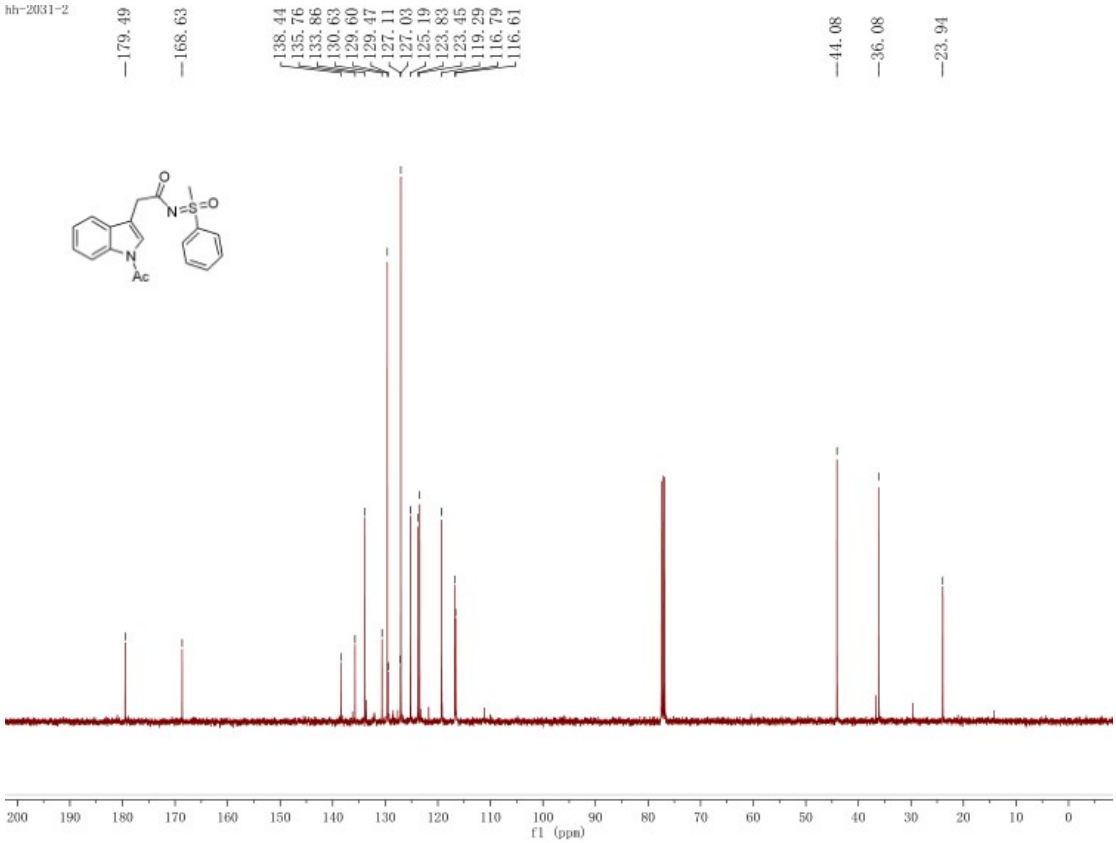
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4z



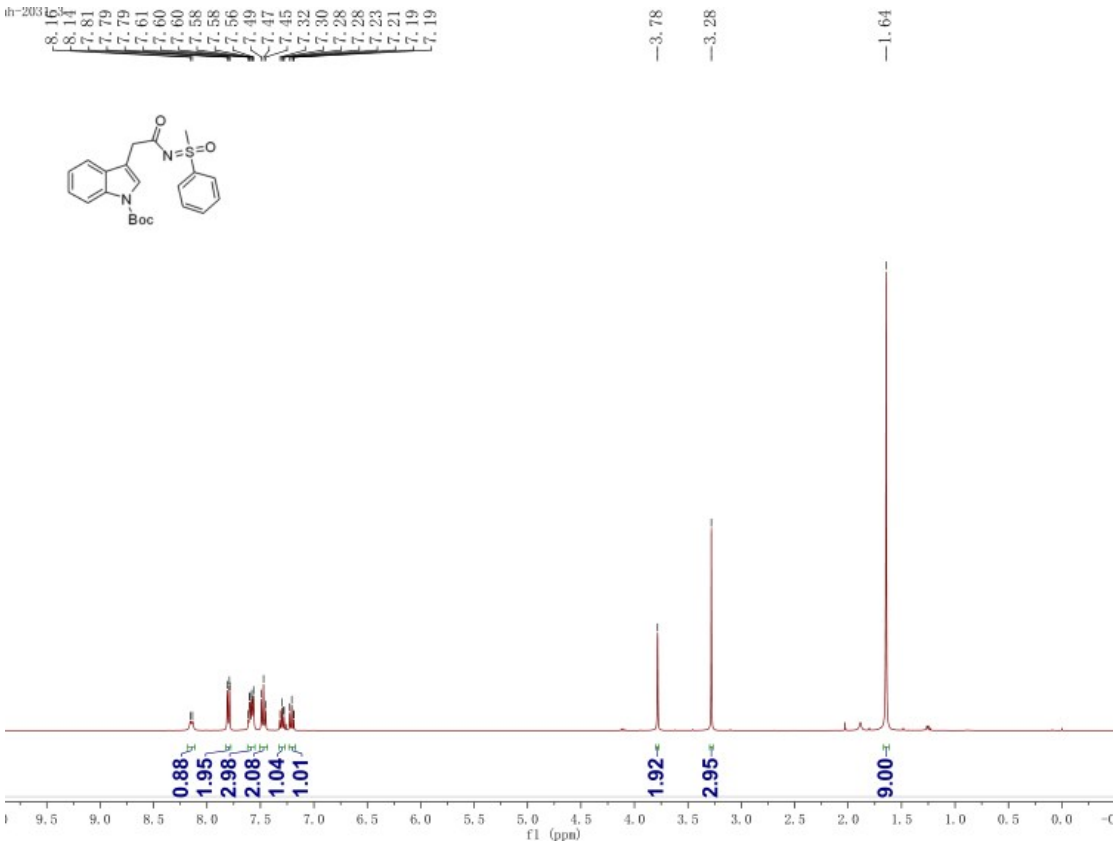
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 6a



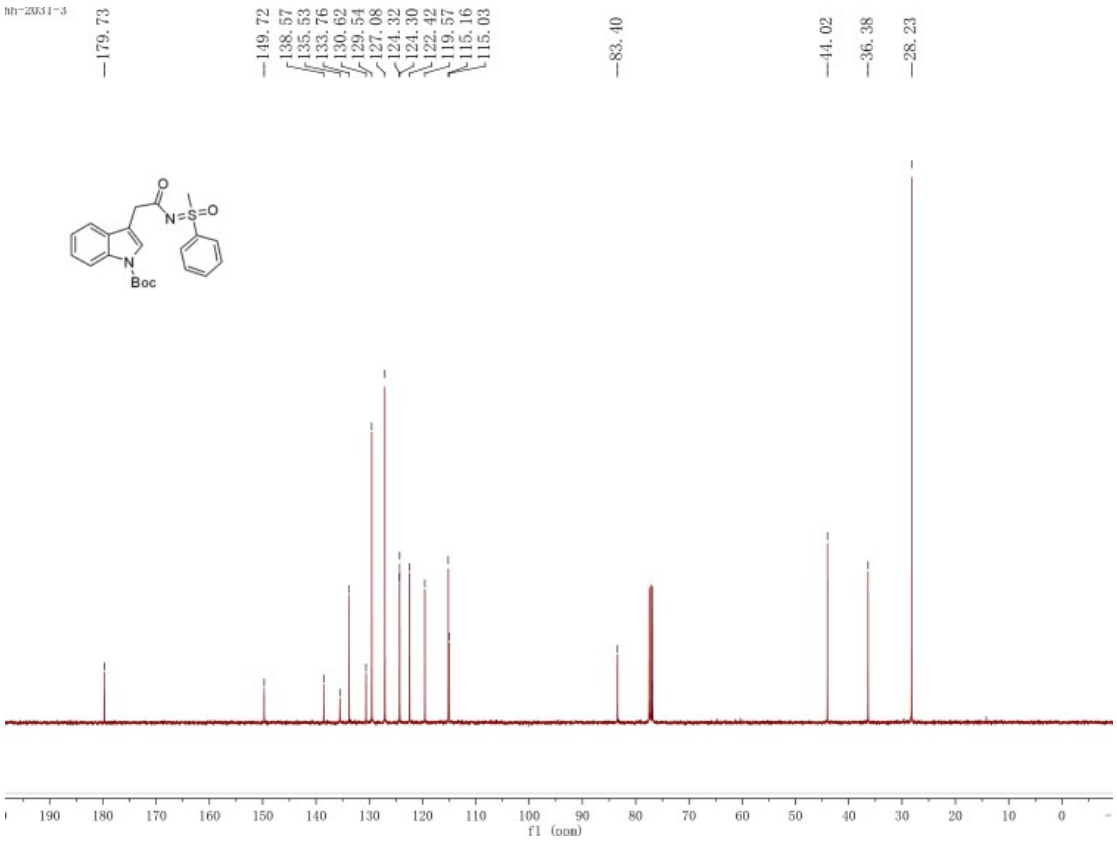
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 6a



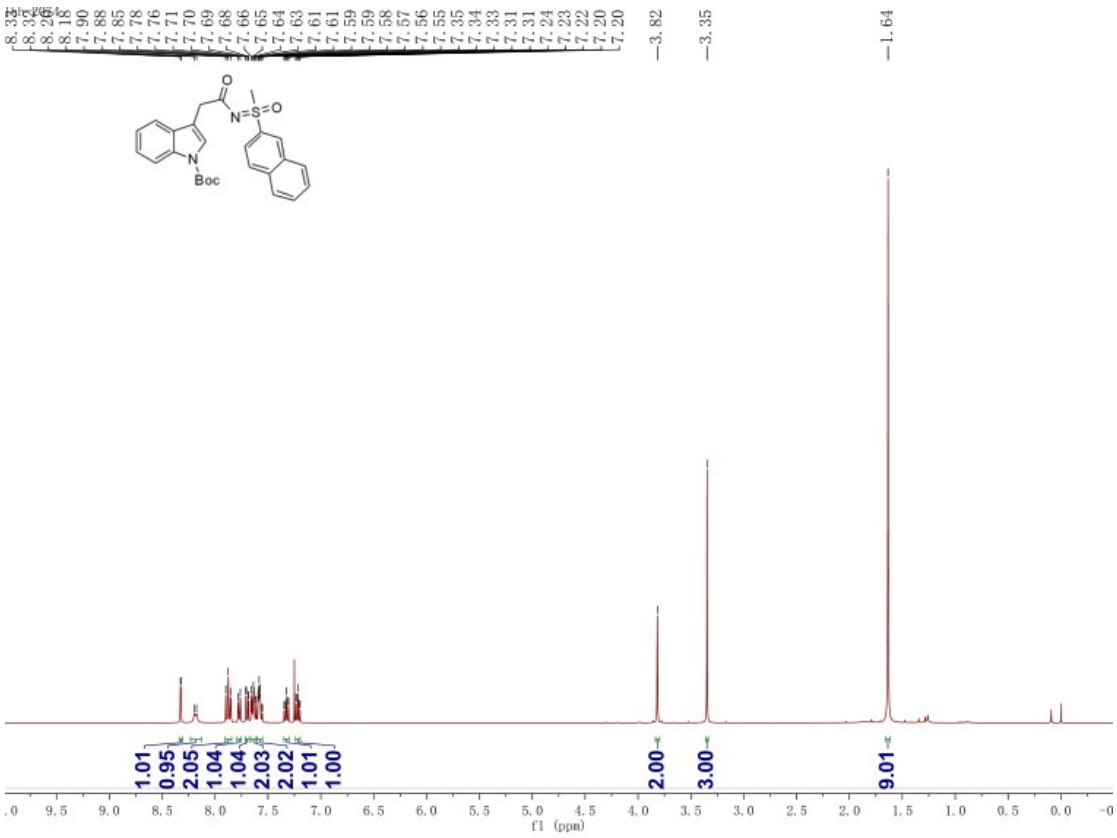
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 6b



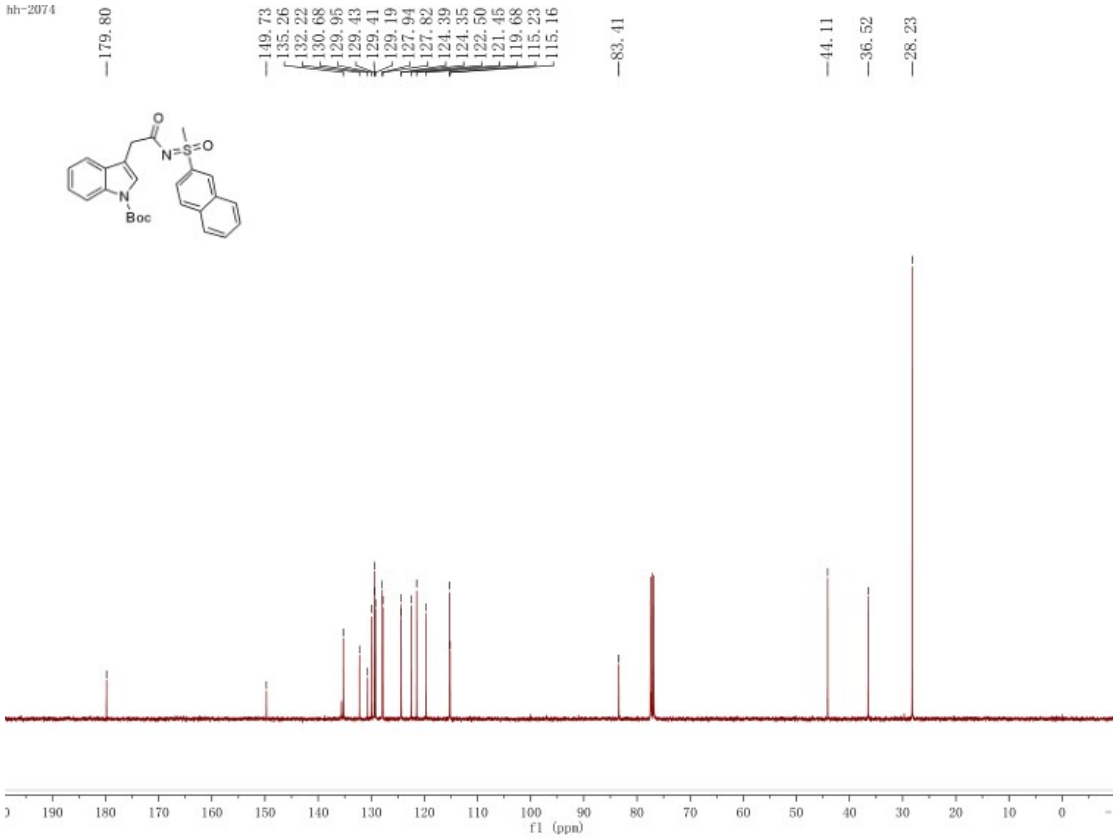
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 6b



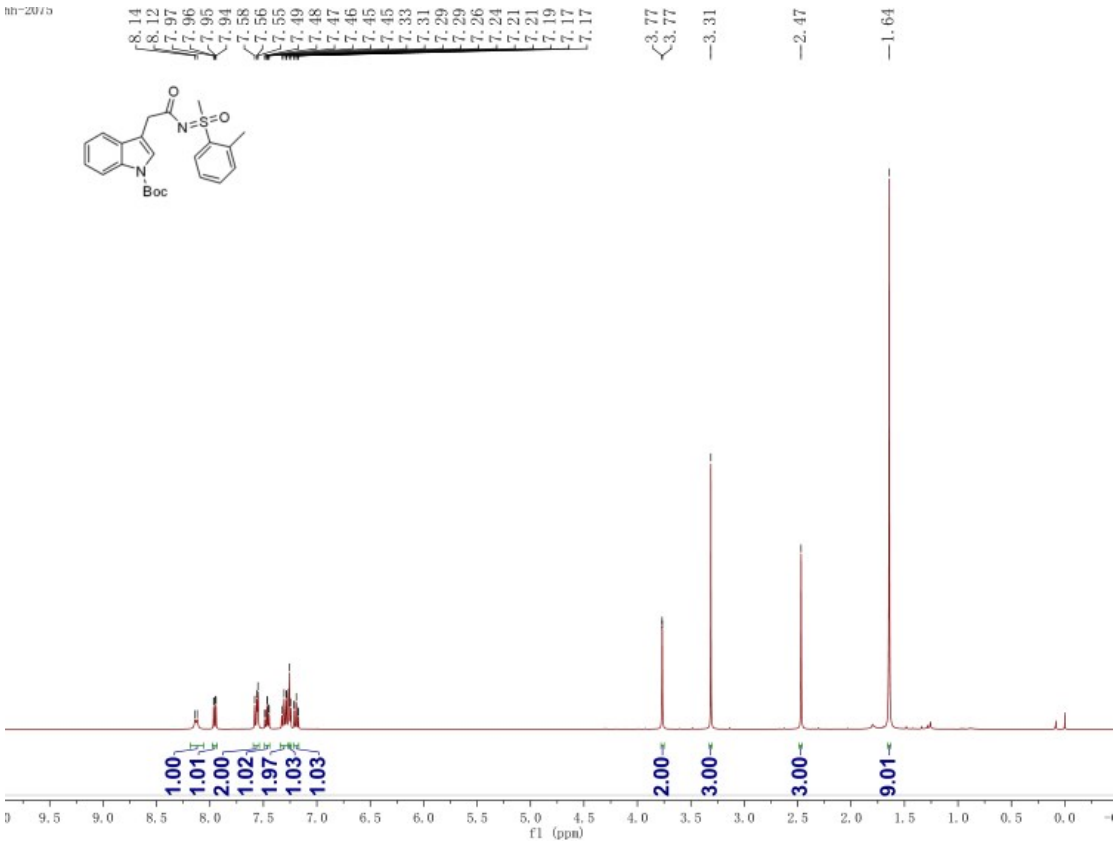
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 6c



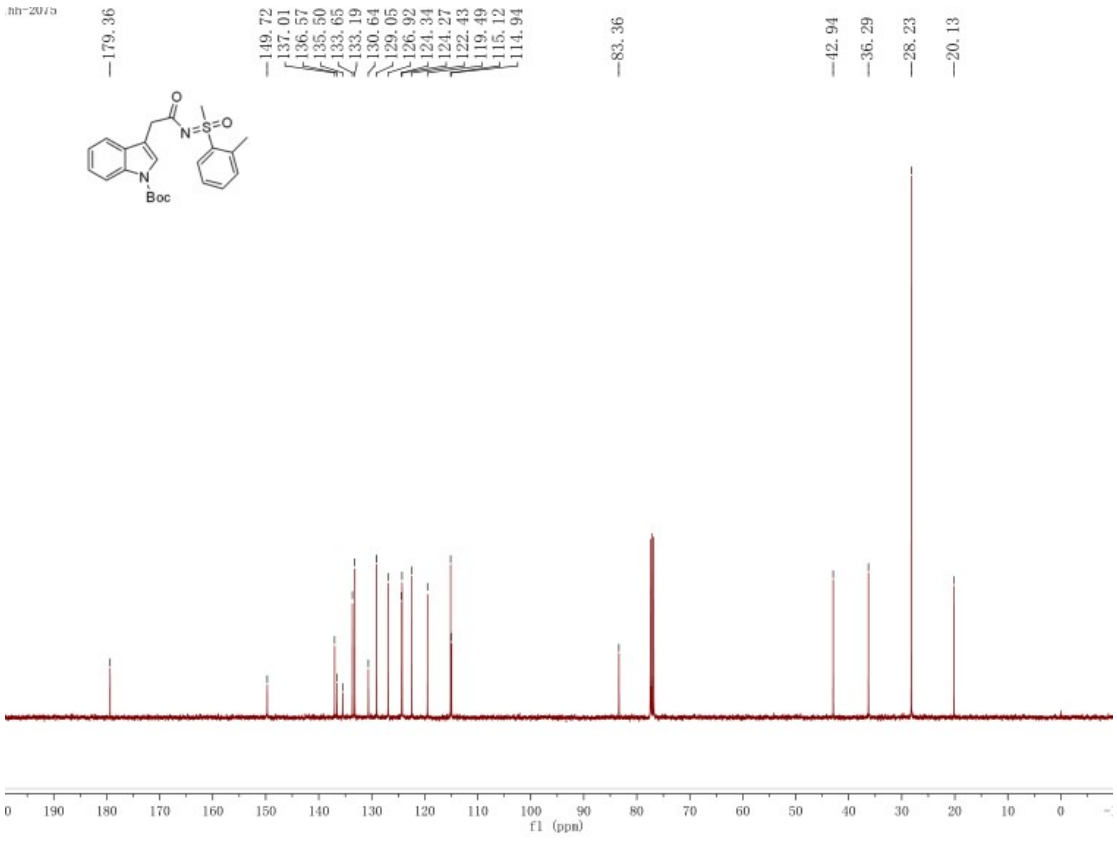
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 6c



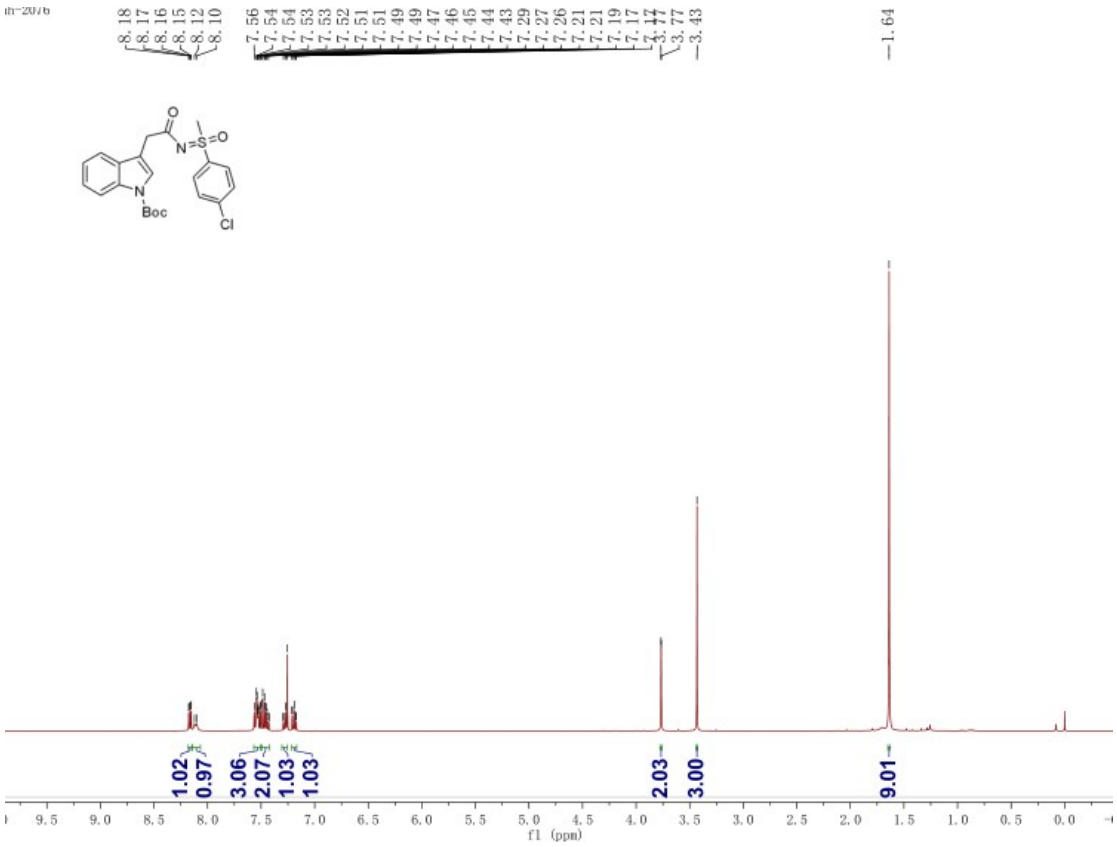
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 6d



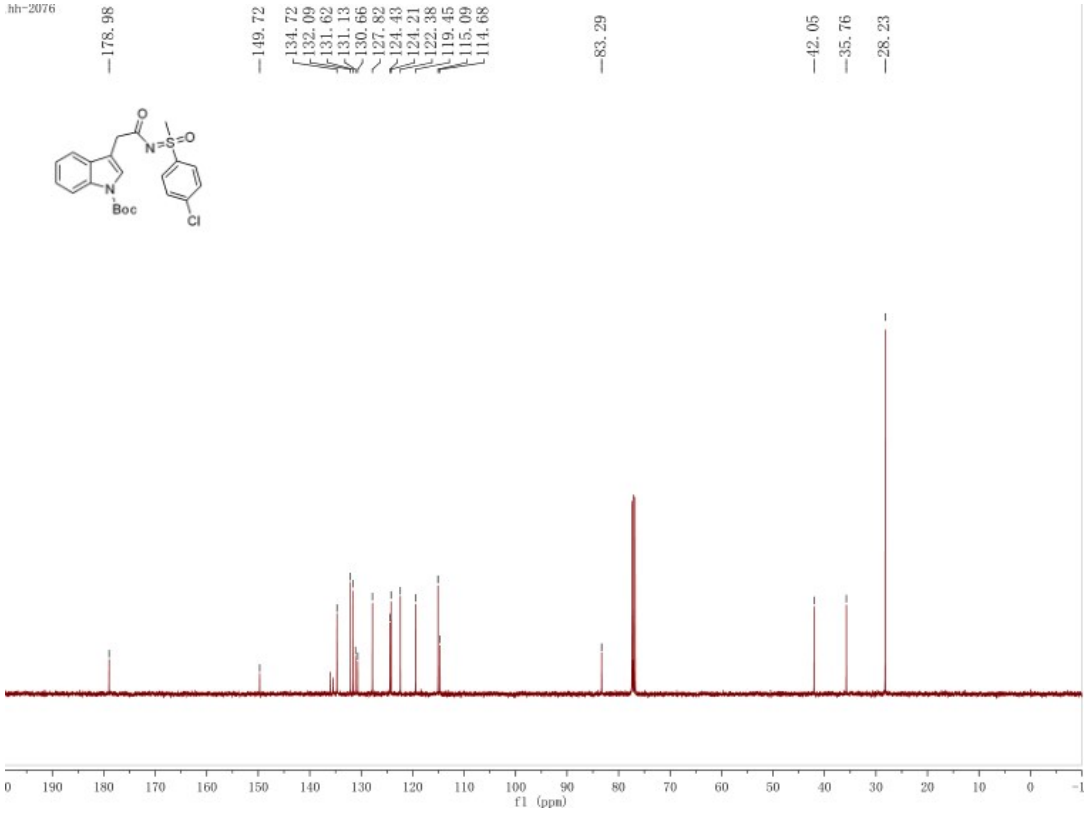
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 6d



^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 6e

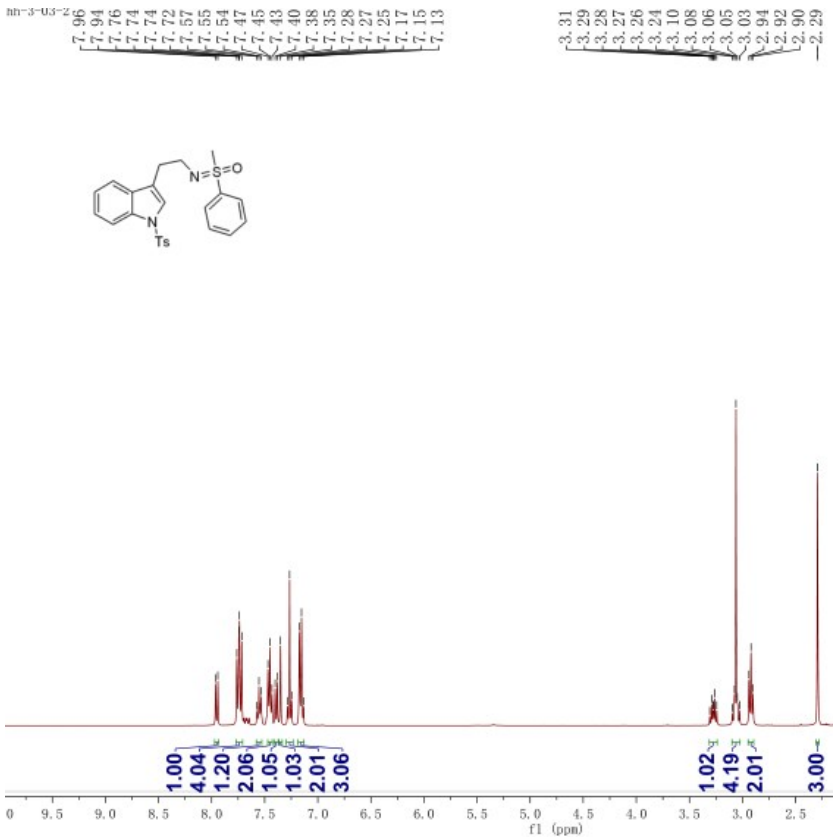


^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 6e

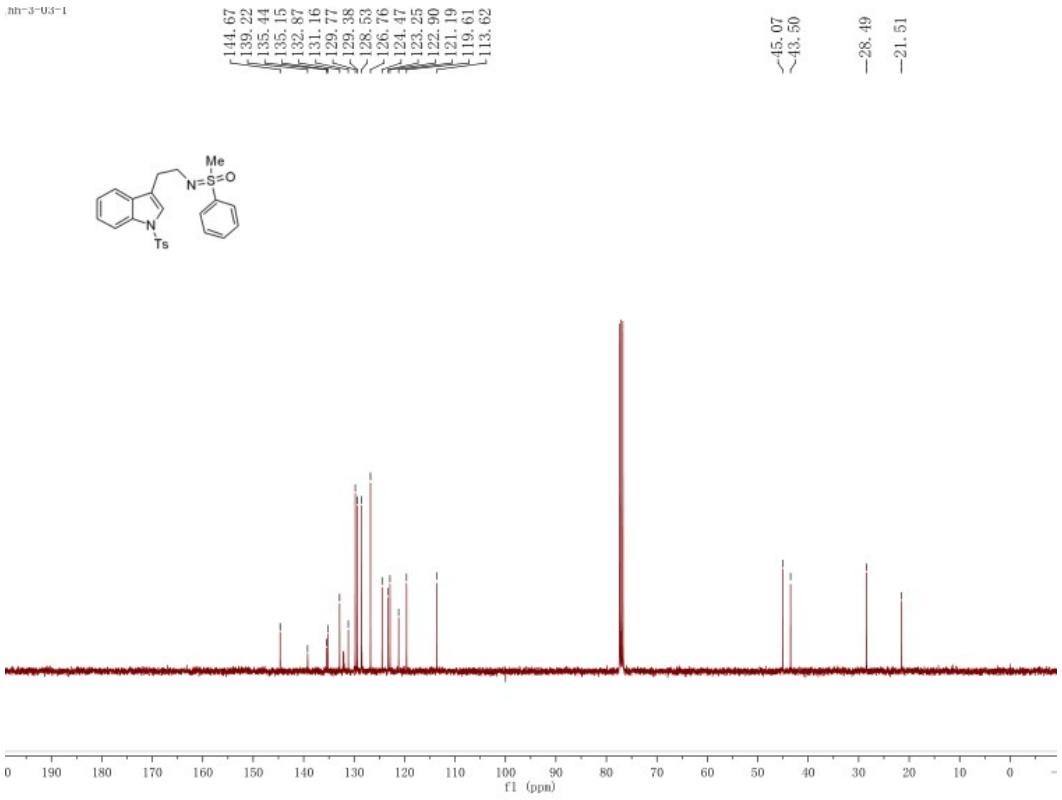


7. ^{1}H and ^{13}C NMR Spectra of compound 8.

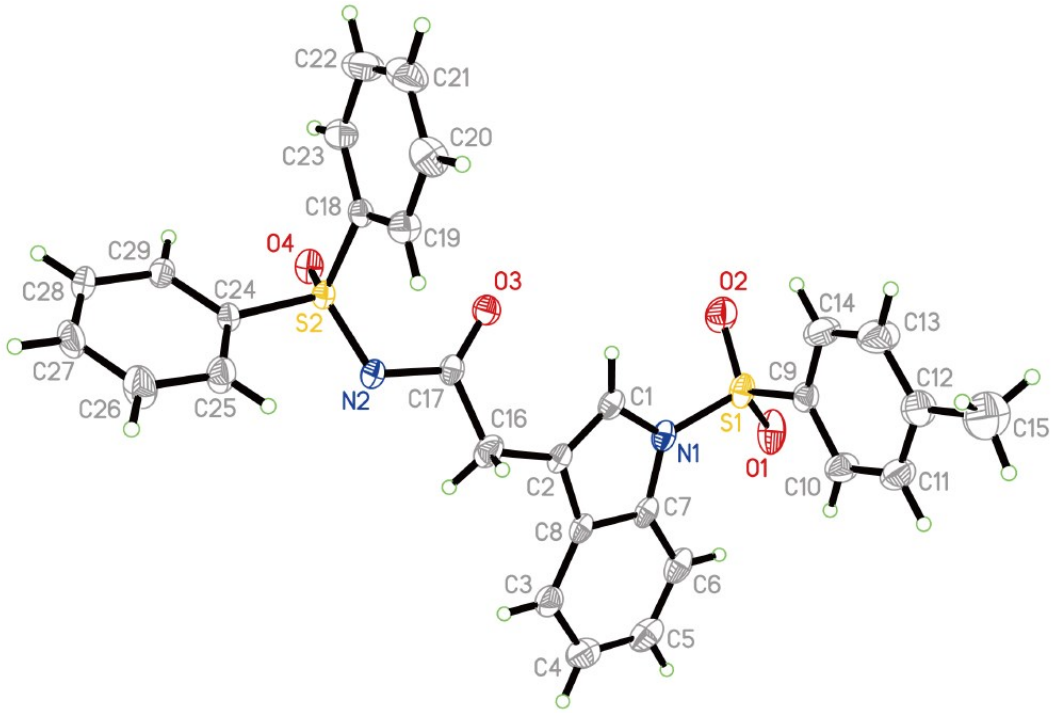
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 8

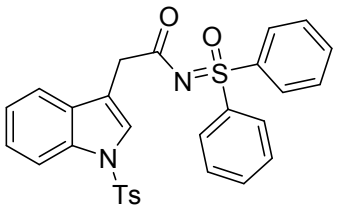


^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 8



8. X-ray crystal structure of compound 4v.





4v

Bond precision: C-C = 0.0033 A Wavelength=0.71073

Cell: a=9.8470(6) b=17.2006(14) c=16.0137(9)
alpha=90 beta=106.046(6) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	2606.6(3)	2606.6(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C29 H24 N2 O4 S2	?
Sum formula	C29 H24 N2 O4 S2	C29 H24 N2 O4 S2
Mr	528.62	528.62
Dx,g cm-3	1.347	1.347
Z	4	4
Mu (mm-1)	0.243	0.243
F000	1104.0	1104.0
F000'	1105.45	
h,k,lmax	11,20,19	11,20,19
Nref	4629	4616
Tmin,Tmax	0.953,0.962	0.953,1.000
Tmin'	0.953	

Correction method= # Reported T Limits: Tmin=0.953 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.095

R(reflections)= 0.0414(4059) wR2(reflections)= 0.1181(4616)

S = 1.003 Npar= 335