Palladium-catalyzed decarboxylative α-allylation of thiazolidinones and azlactones with sulfonamido-substituted acyclic allylic carbonates

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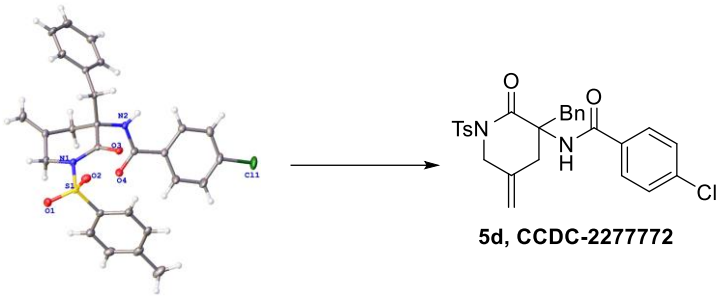
Supporting Information

Table of Contents

1. X-Ray crystal data for compound 5d

Single crystal of compound **5d** was prepared from the mixture solvent of EtOH and CH_2Cl_2. A suitable crystal was selected for structure determination on a Xcalibur, Eos, Gemini diffractometer. The crystal was kept at 293(2) K during data collection. Using Olex2, the structure was solved with the ShelXS structure solution program using Direct Methods and refined with the ShelXLrefinement package using Least Squares minimisation.



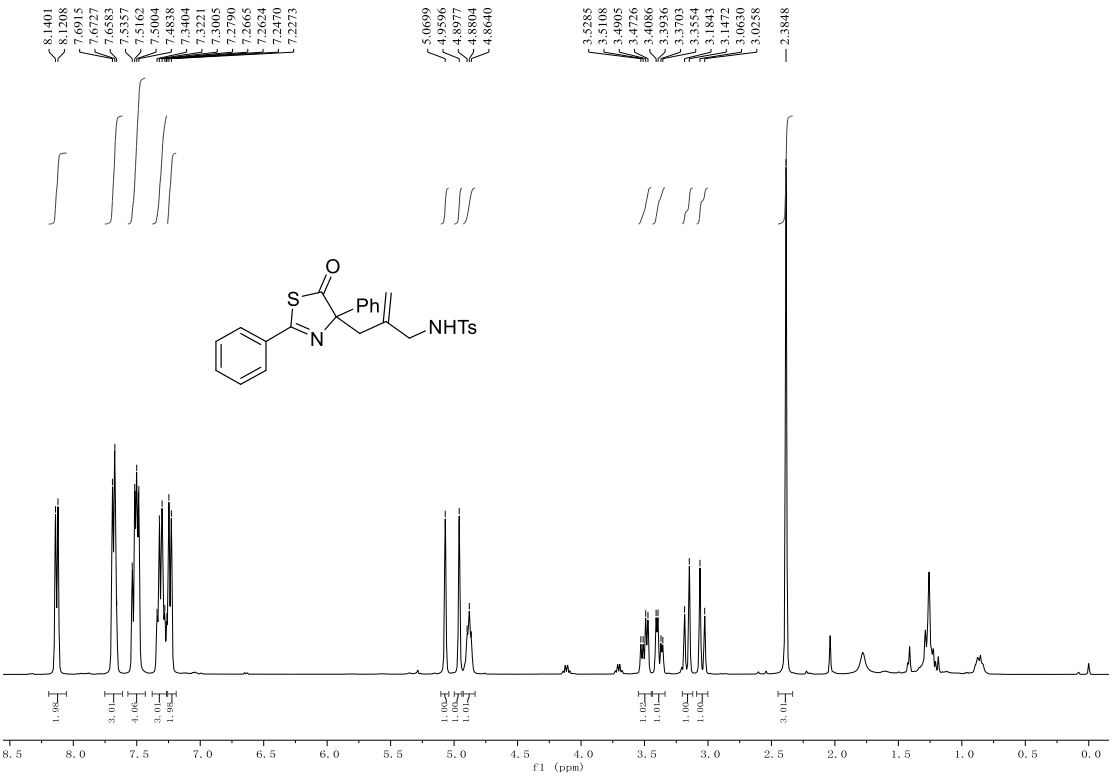
ORTEP of **5d** (at 50% level)

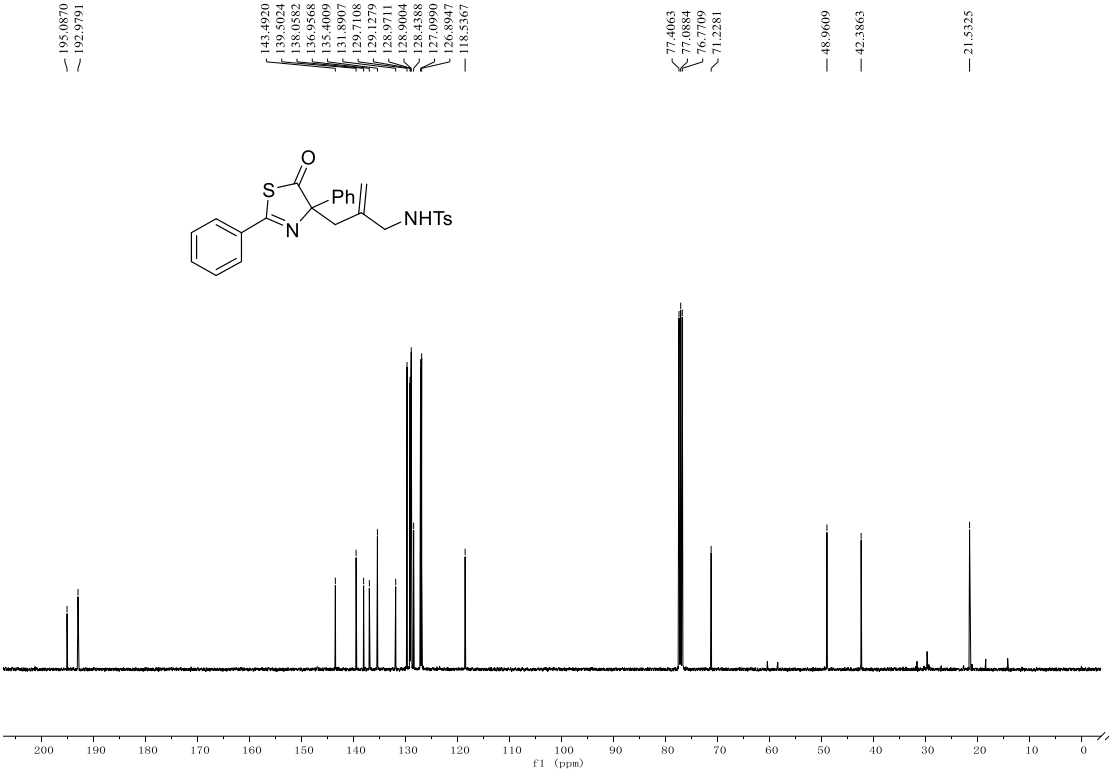
Crystal data and structure refinement for 5d (CCDC-2277772)

Identification code	**5d**
Empirical formula	$C_{27}H_{25}ClN_2O_4S$
Formula weight	509.00
Temperature/K	99.98(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.1642(2)
b/Å	11.1077(2)
c/Å	12.6071(2)
α/°	67.633(2)
β/°	85.5240(10)
γ/°	70.287(2)
Volume/Å^3	1237.06(4)
Z	2
ρ_{calc}g/cm^3	1.366
μ/mm^{-1}	2.460
F(000)	532.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.596 to 143.032
Index ranges	$-12 \le h \le 10$, $-13 \le k \le 13$, $-15 \le l \le 15$
Reflections collected	12363
Independent reflections	4679 [R_{int} = 0.0207, R_{sigma} = 0.0184]
Data/restraints/parameters	4679/0/329
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0365, wR_2 = 0.0976
Final R indexes [all data]	R_1 = 0.0373, wR_2 = 0.0982
Largest diff. peak/hole / e Å^{-3}	0.34/-0.54

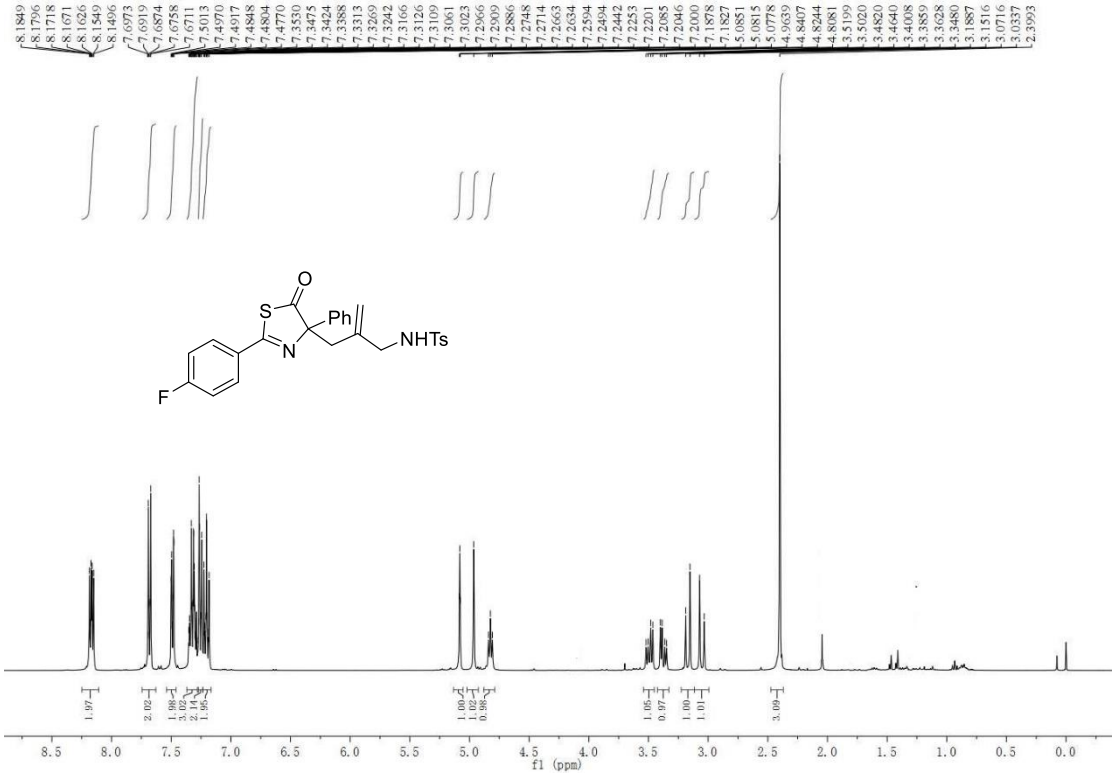
2. ^{1}H and ^{13}C NMR spectra for compounds 3 and 5

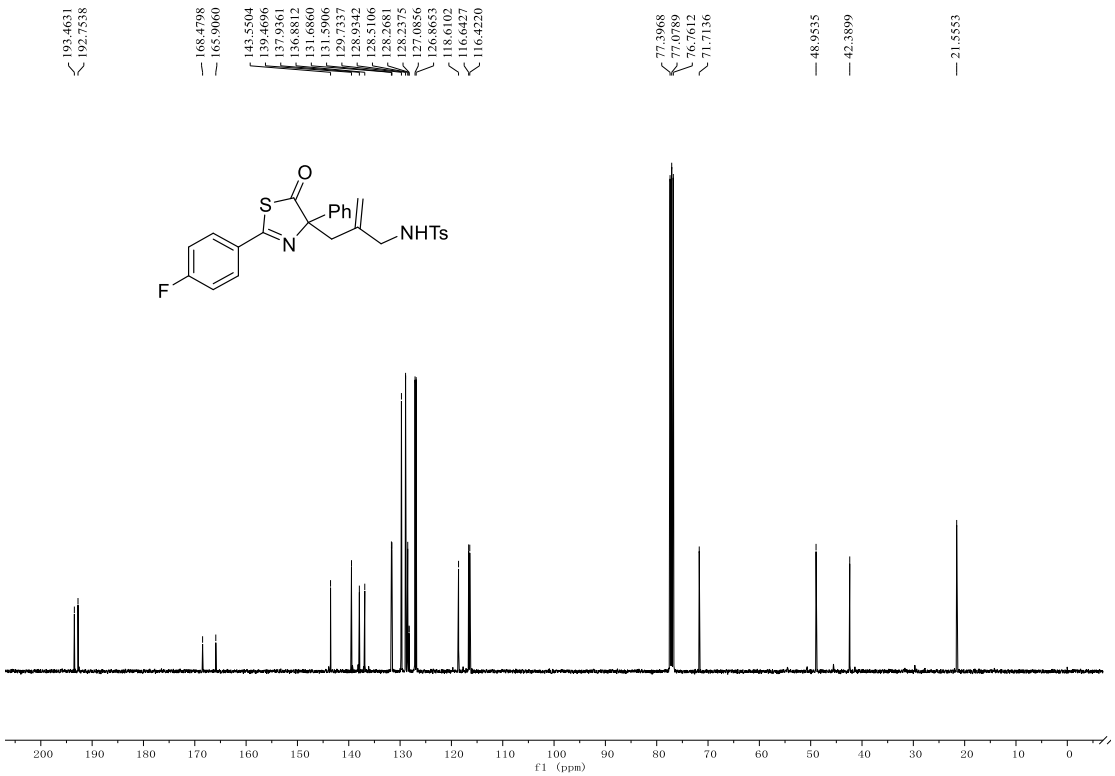
^{1}H and ^{13}C NMR spectra for compound 3a



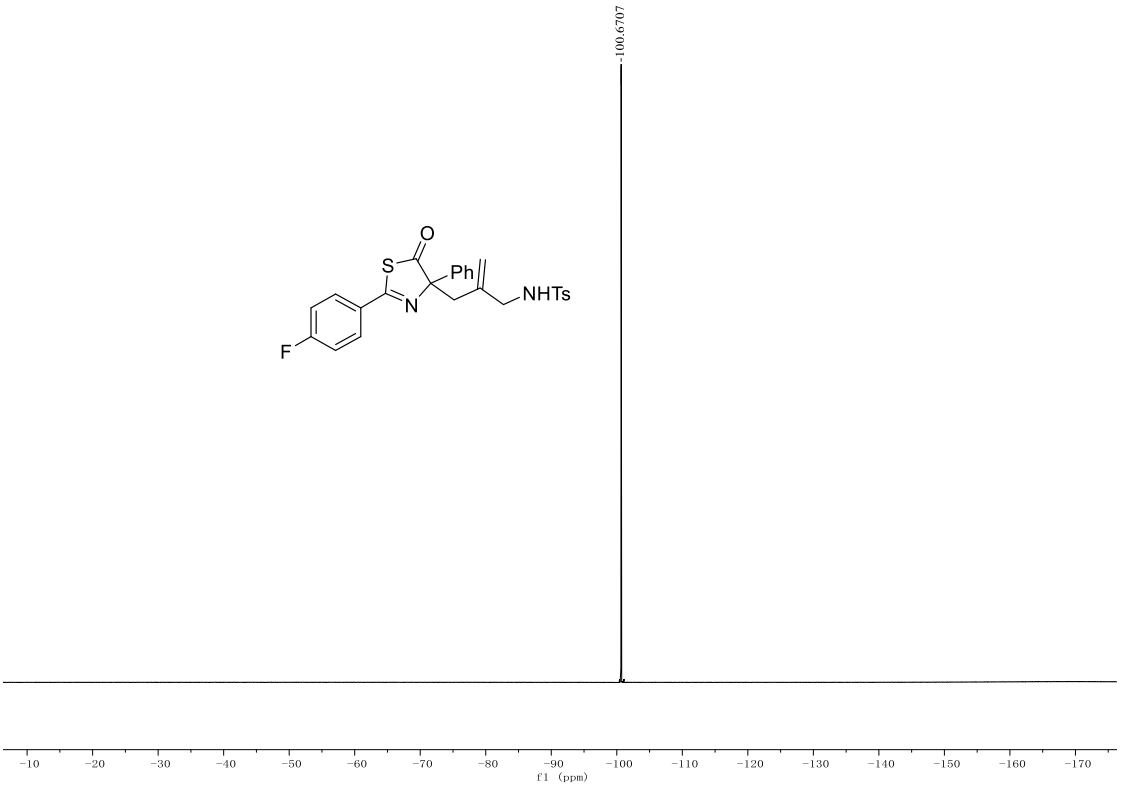


^{1}H and ^{13}C NMR spectra for compound 3b

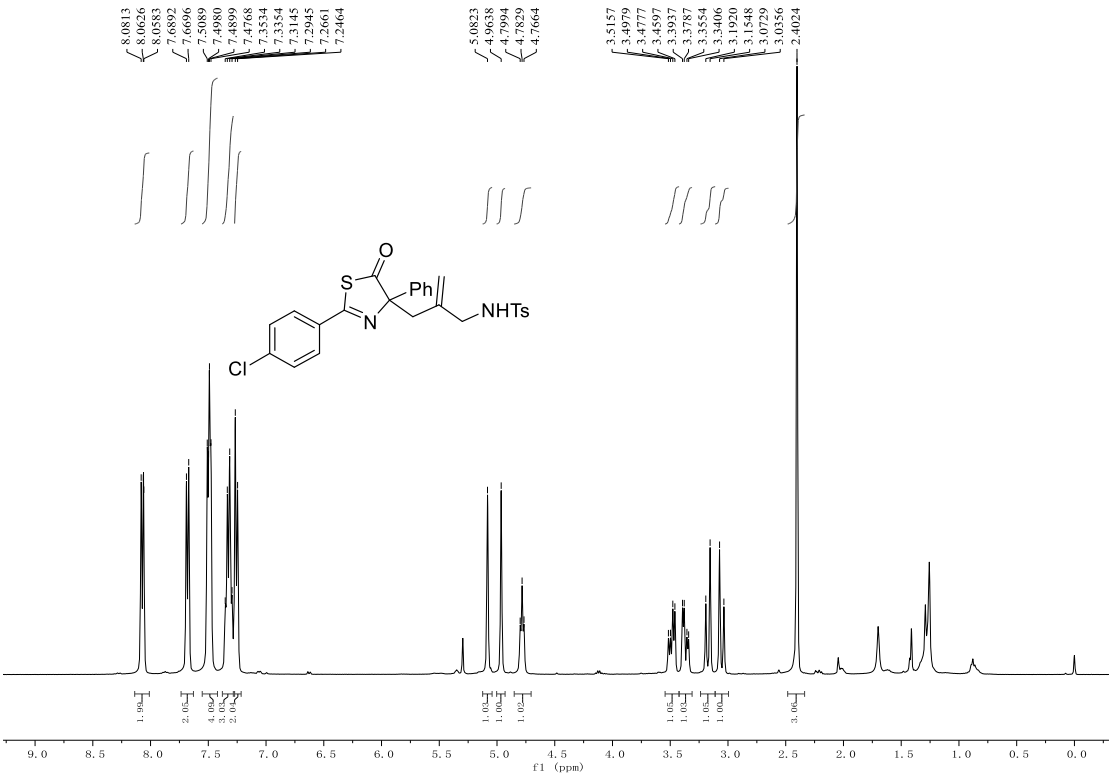


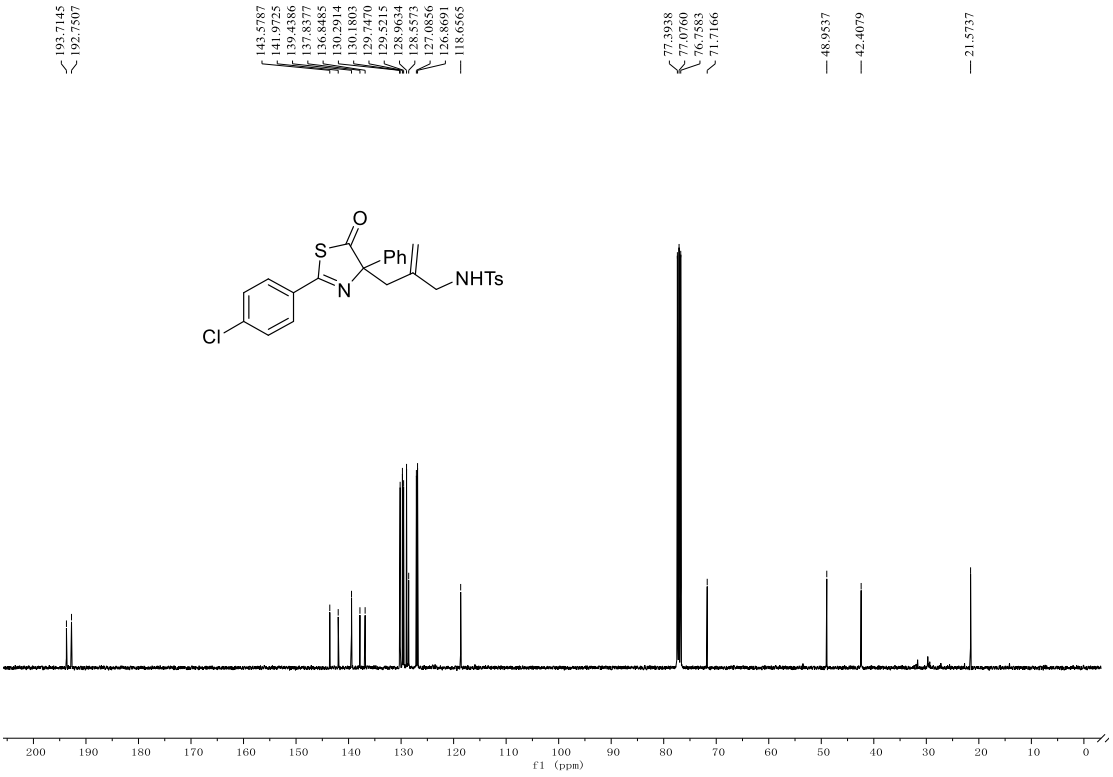


^{19}F NMR spectra for compound 3b

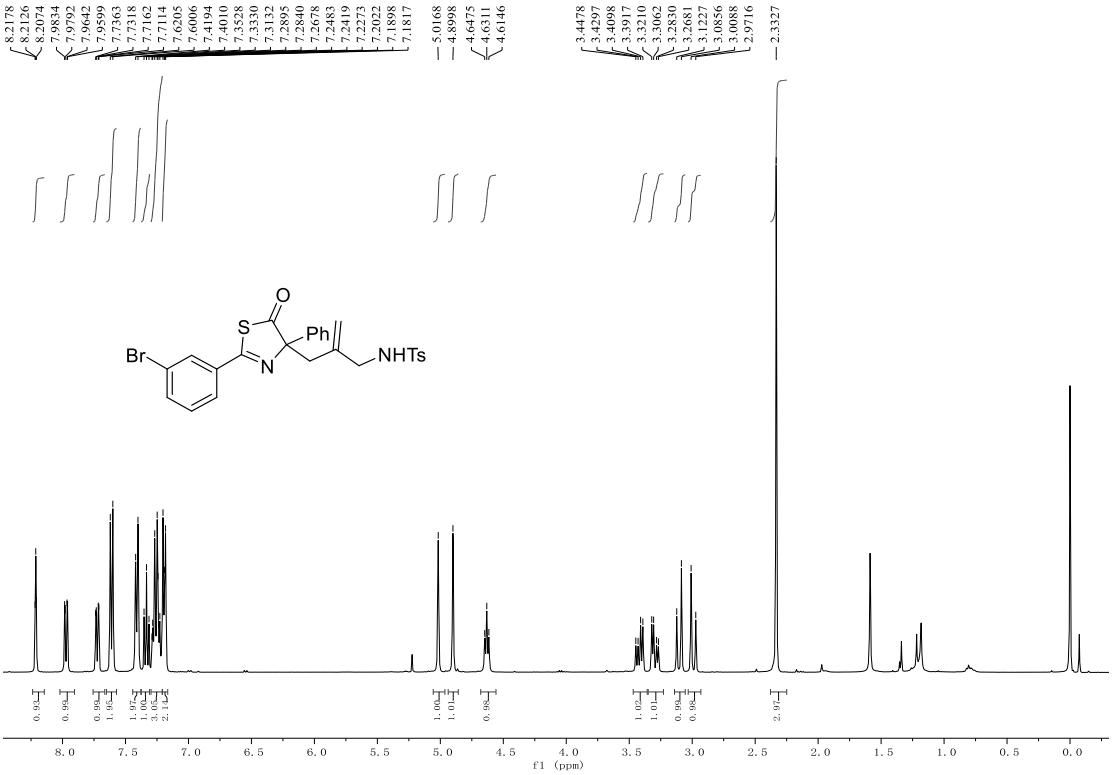


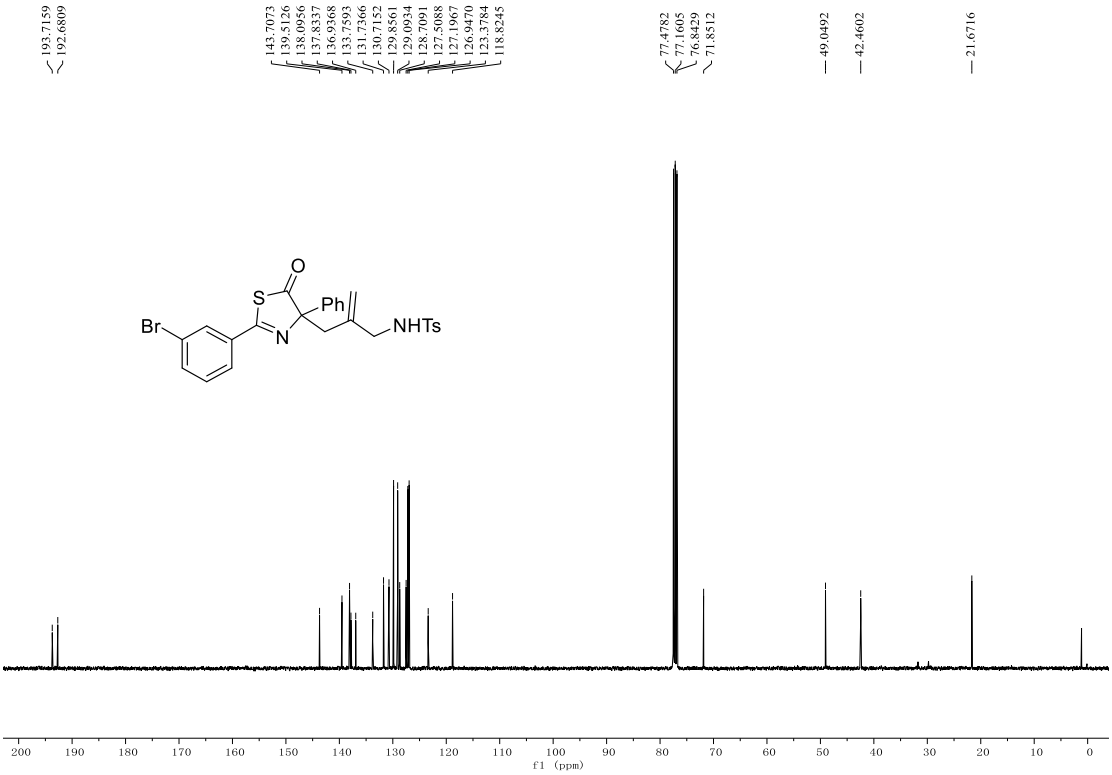
^{1}H and ^{13}C NMR spectra for compound 3c



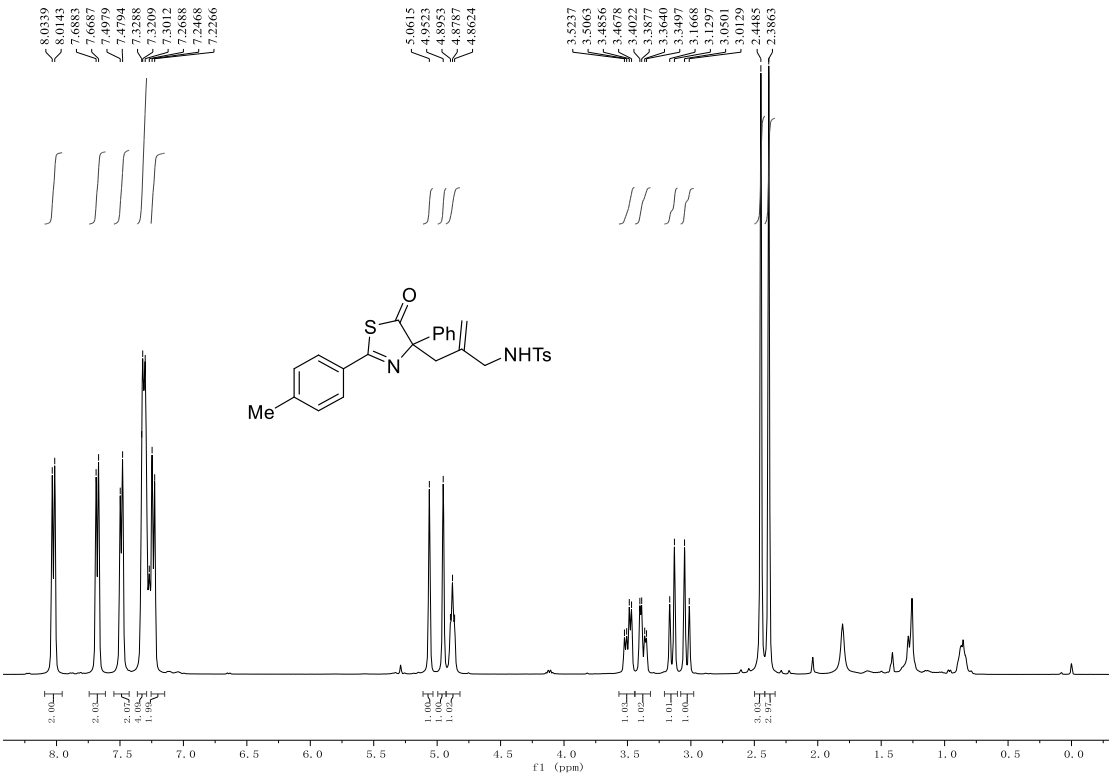


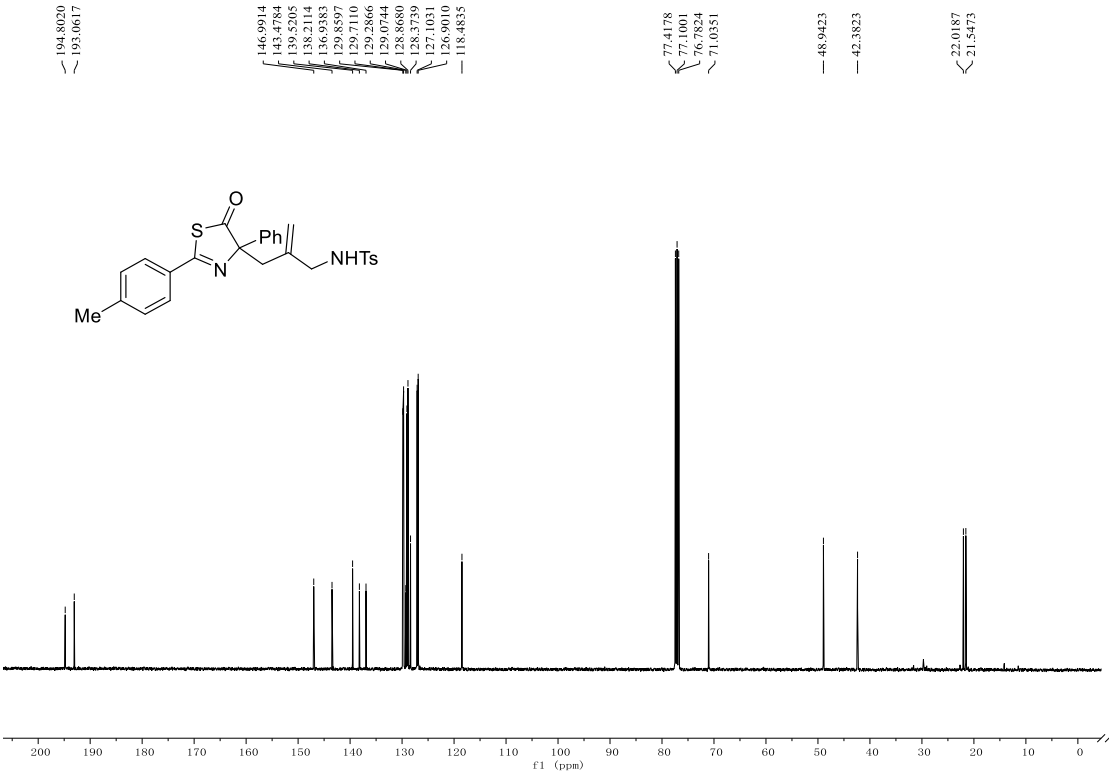
^{1}H and ^{13}C NMR spectra for compound 3d



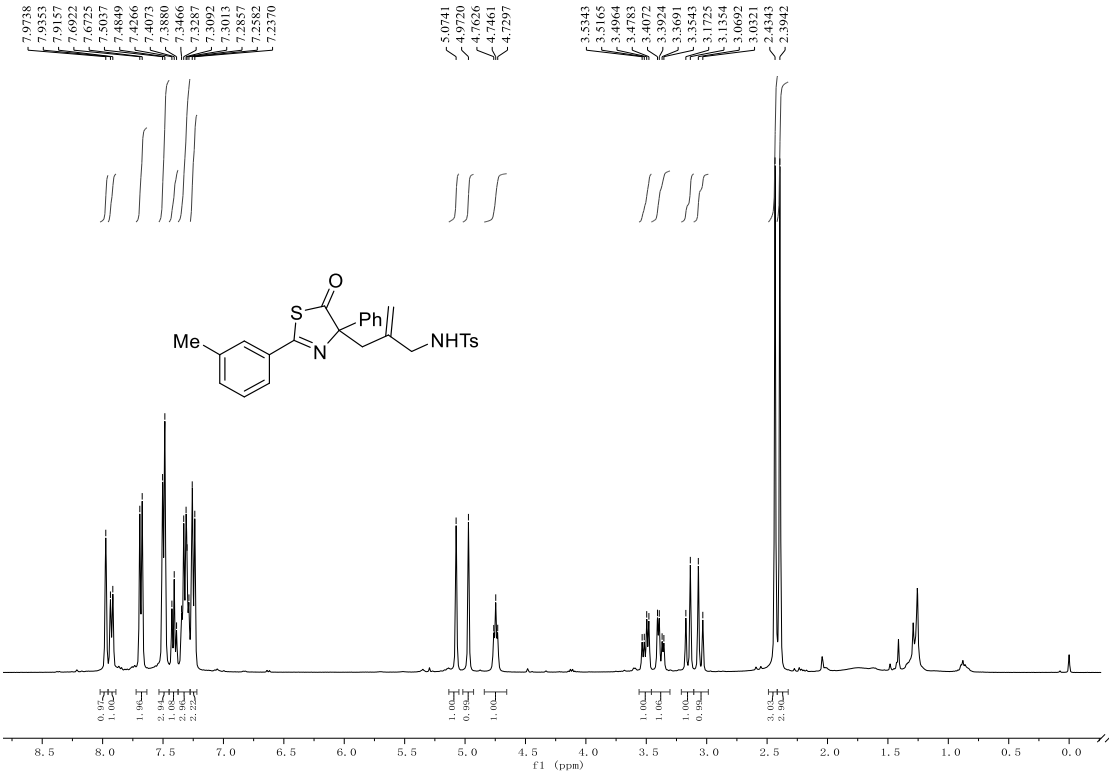


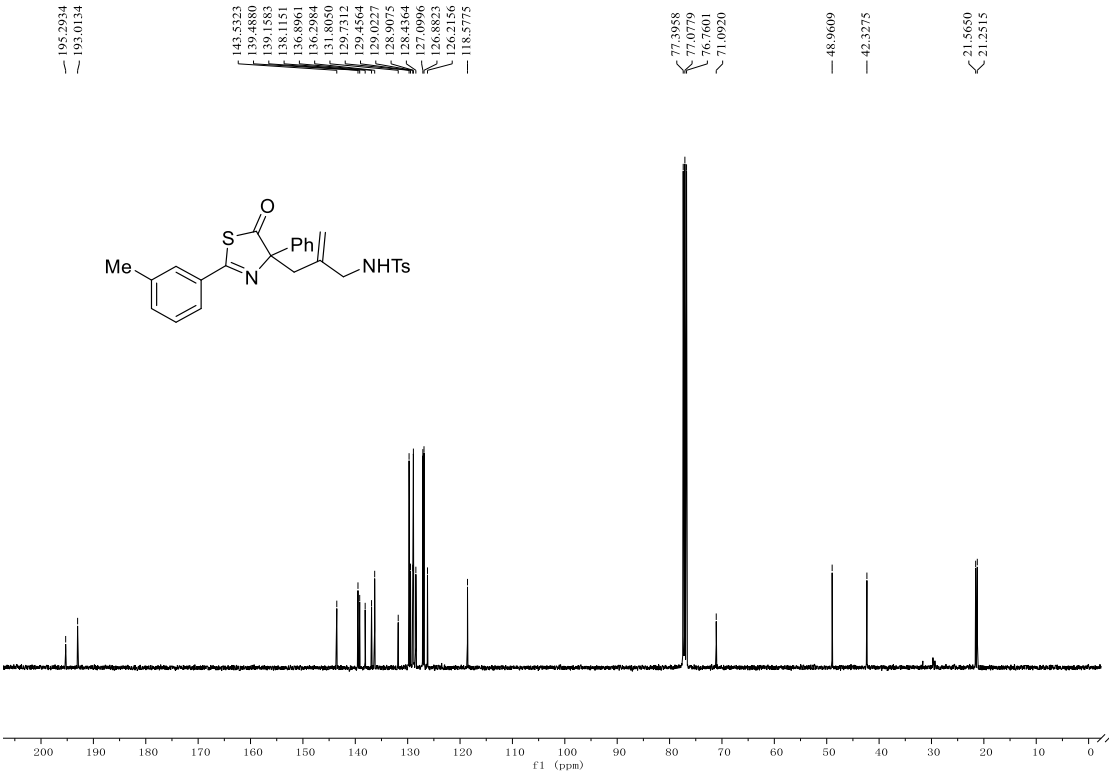
^{1}H and ^{13}C NMR spectra for compound 3e



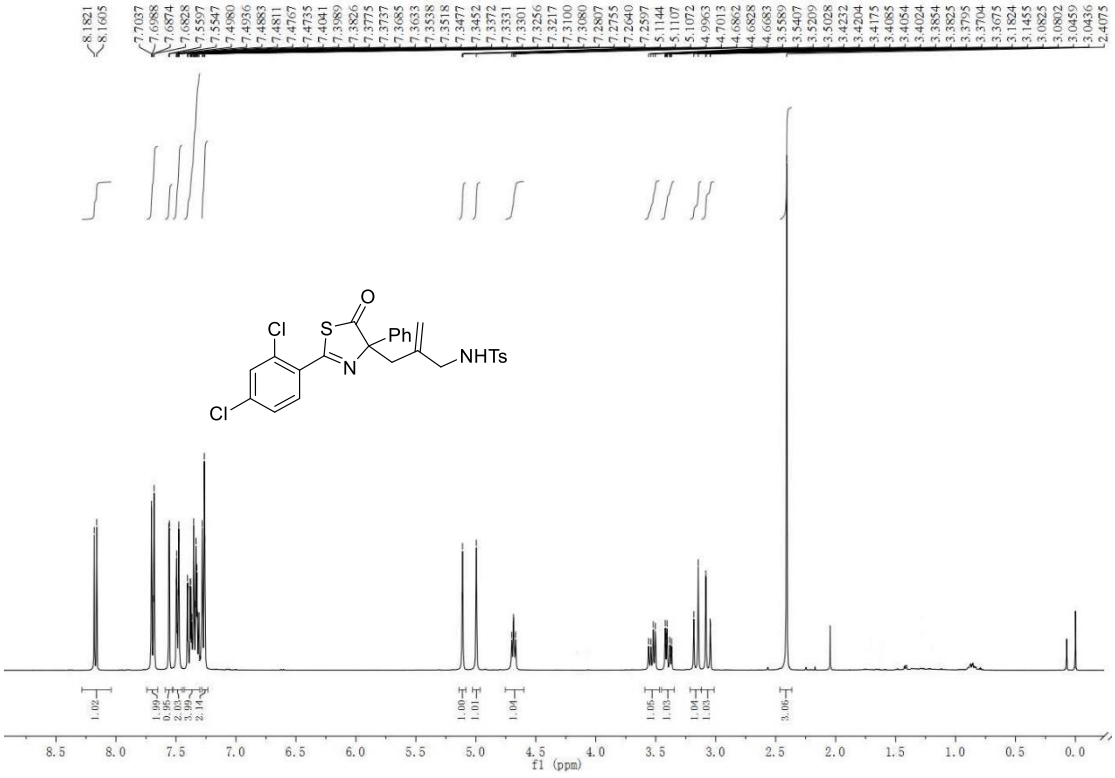


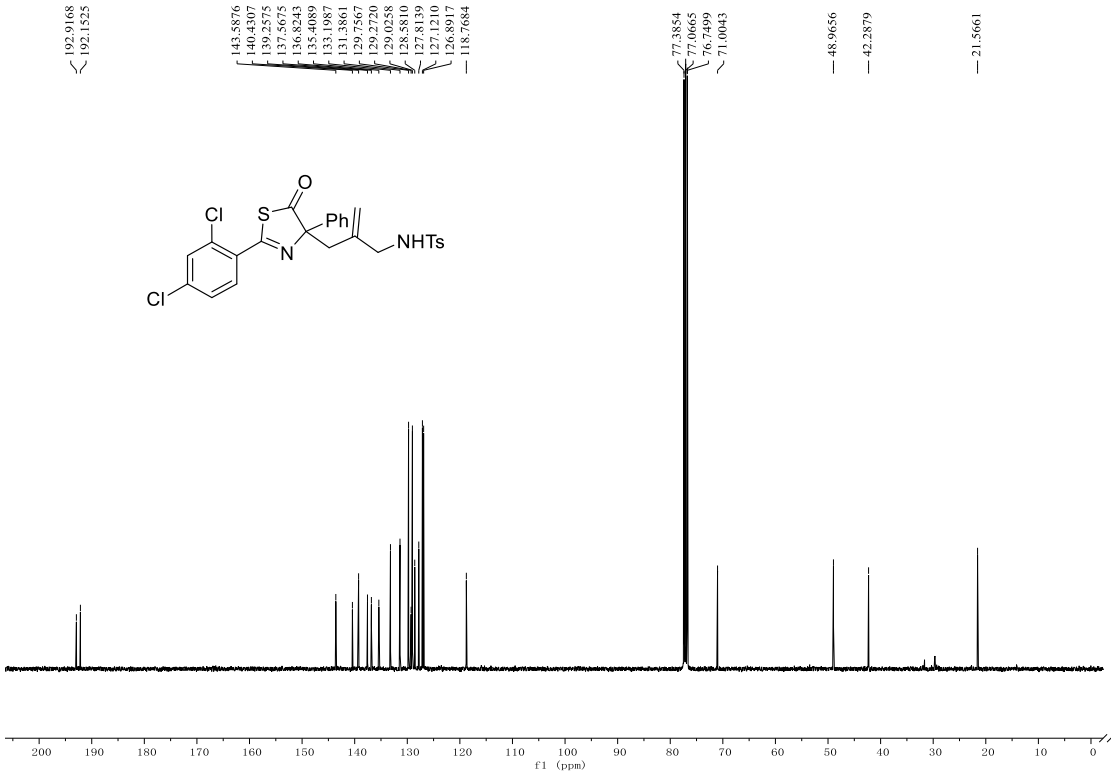
^{1}H and ^{13}C NMR spectra for compound 3f



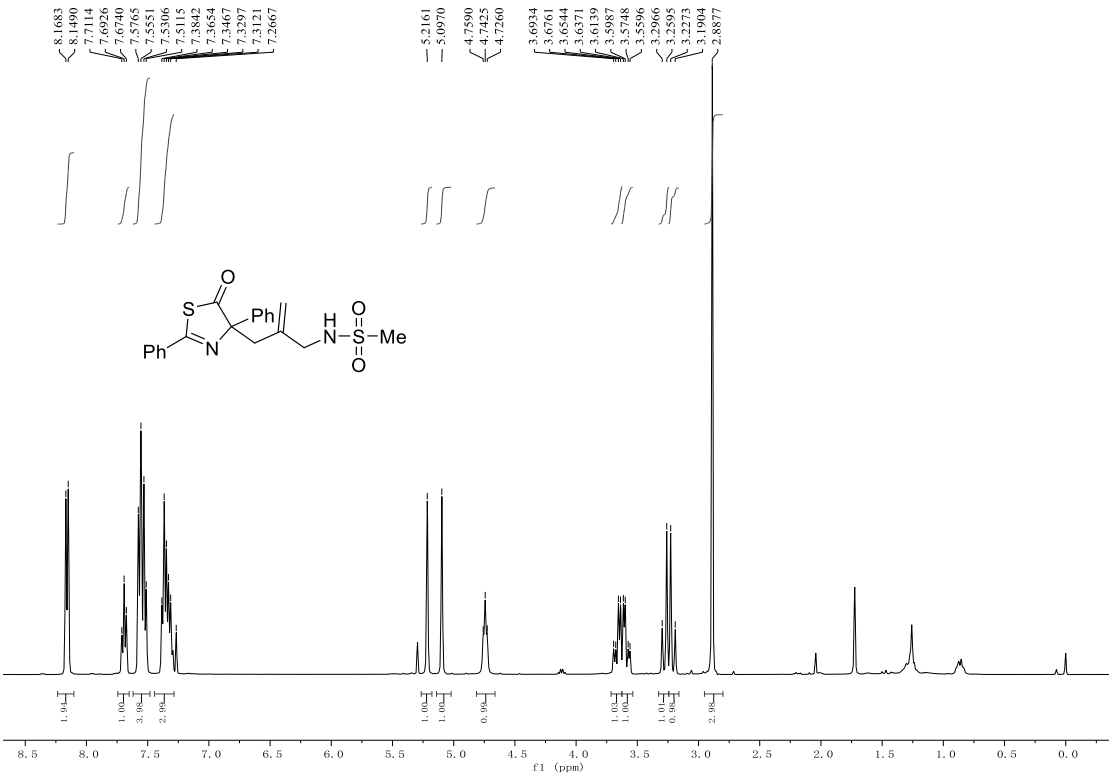


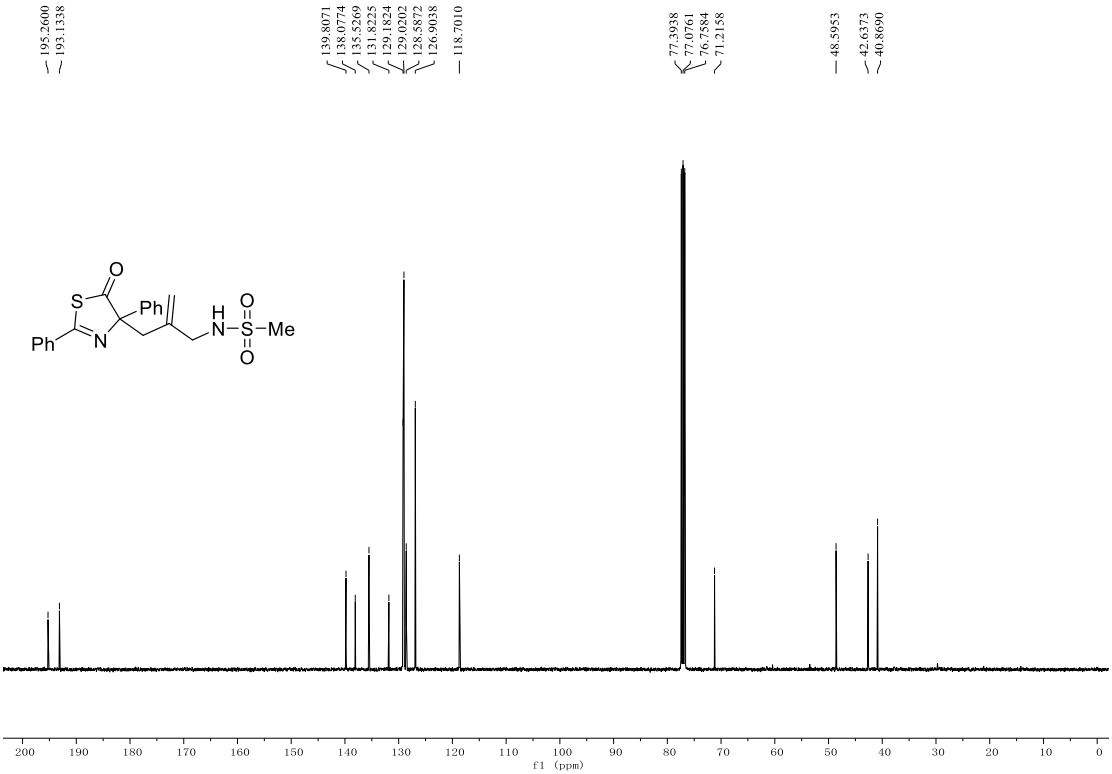
^{1}H and ^{13}C NMR spectra for compound 3g



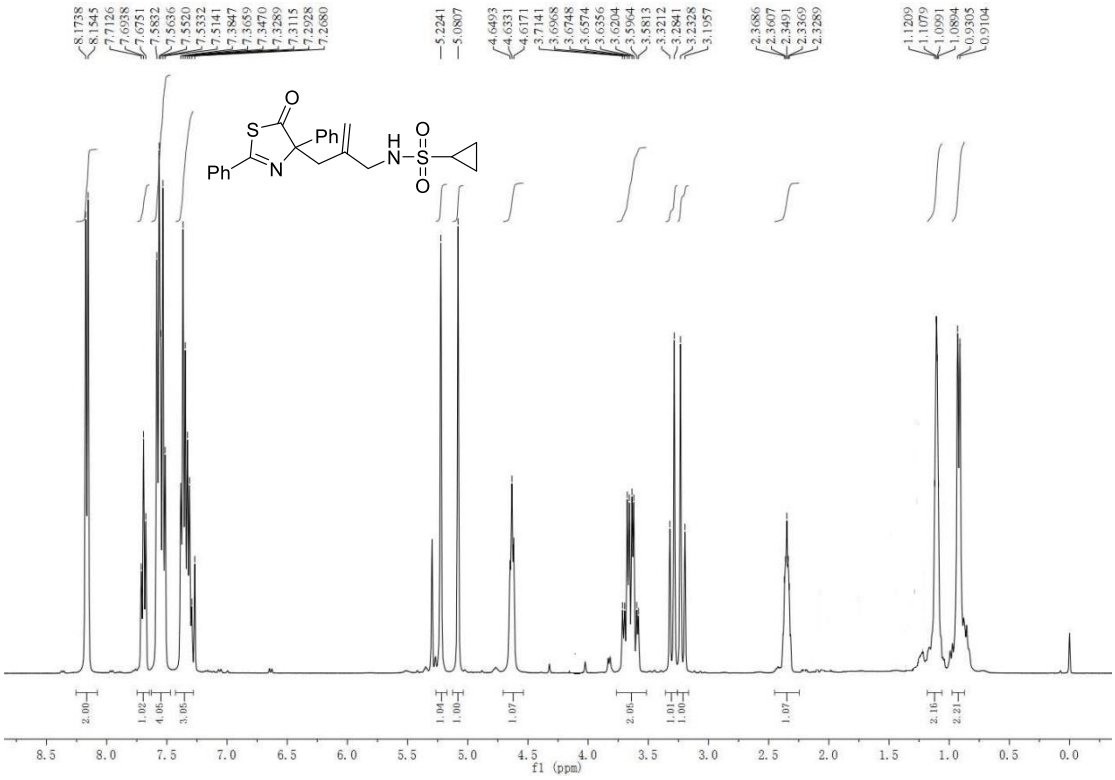


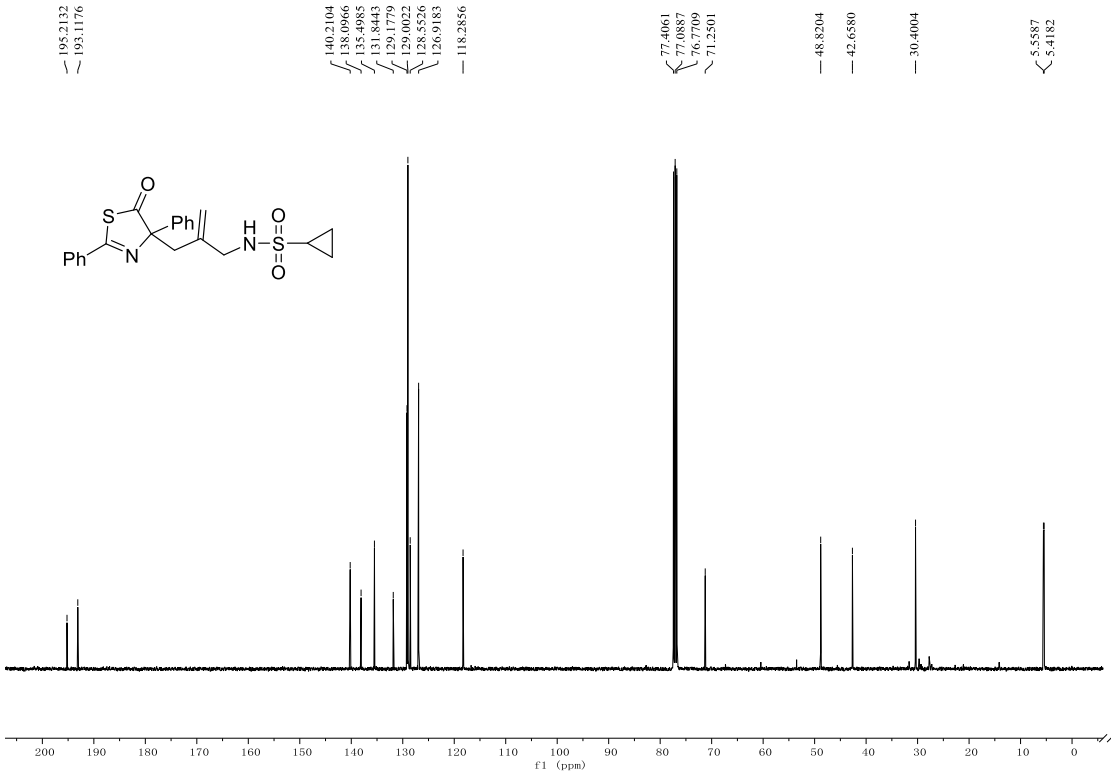
^{1}H and ^{13}C NMR spectra for compound 3h



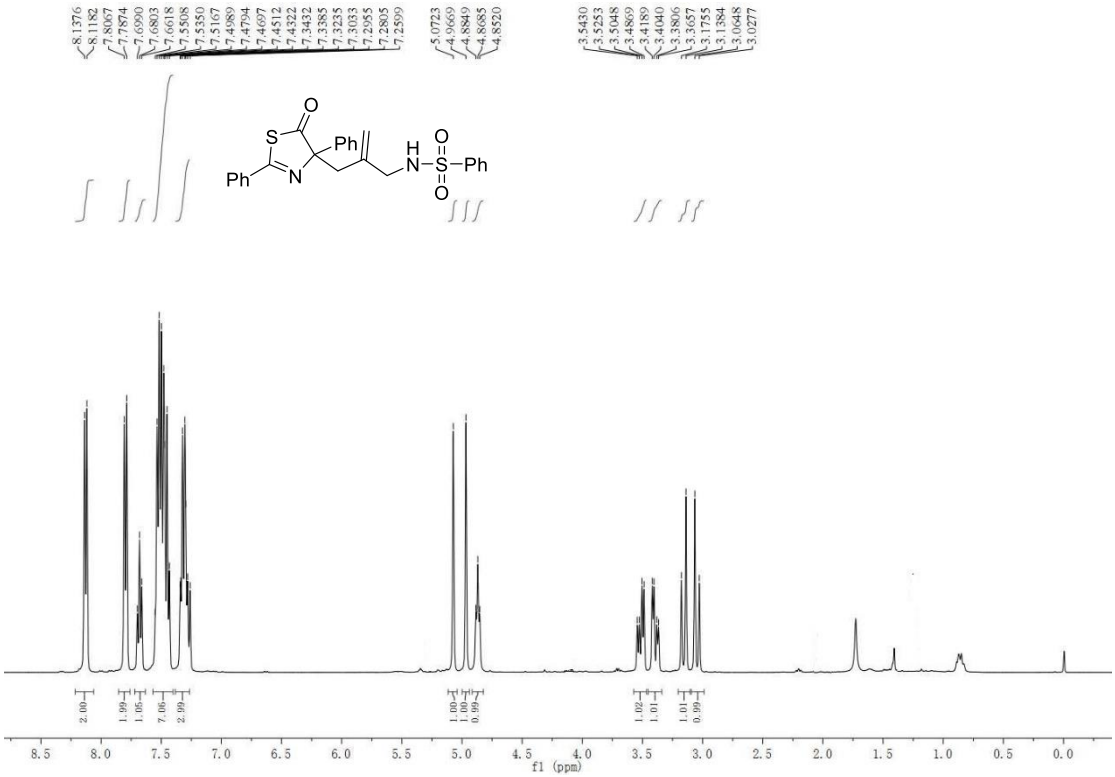


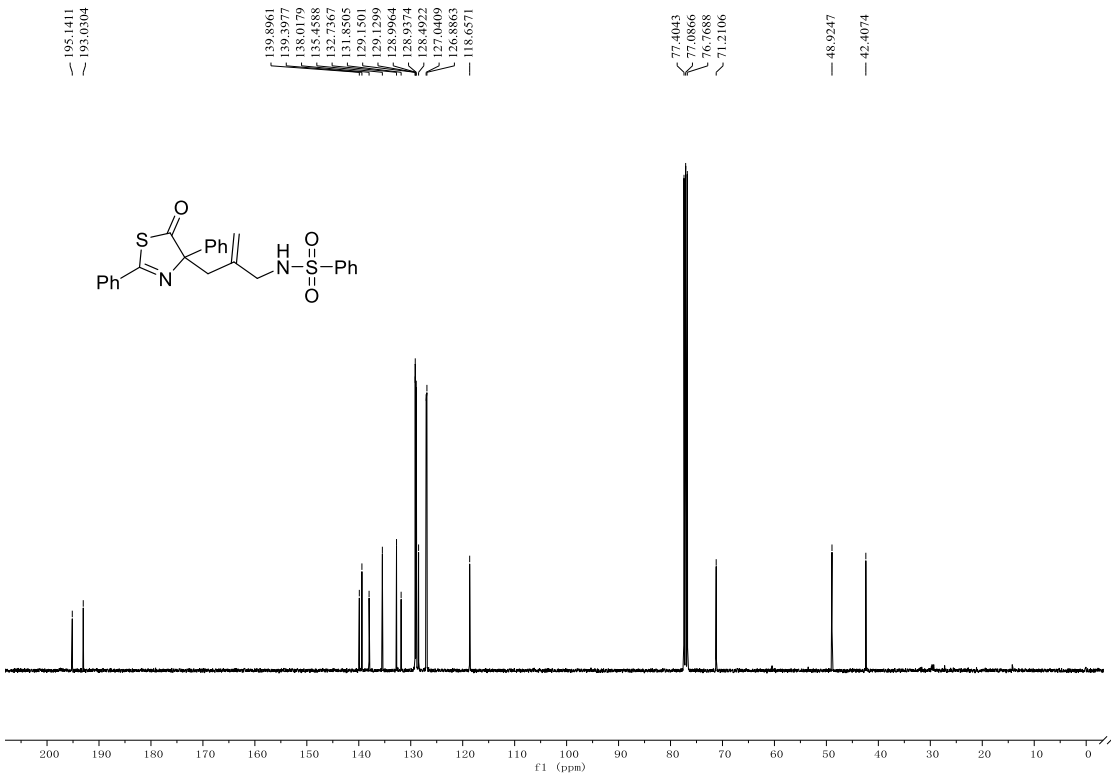
^{1}H and ^{13}C NMR spectra for compound 3i



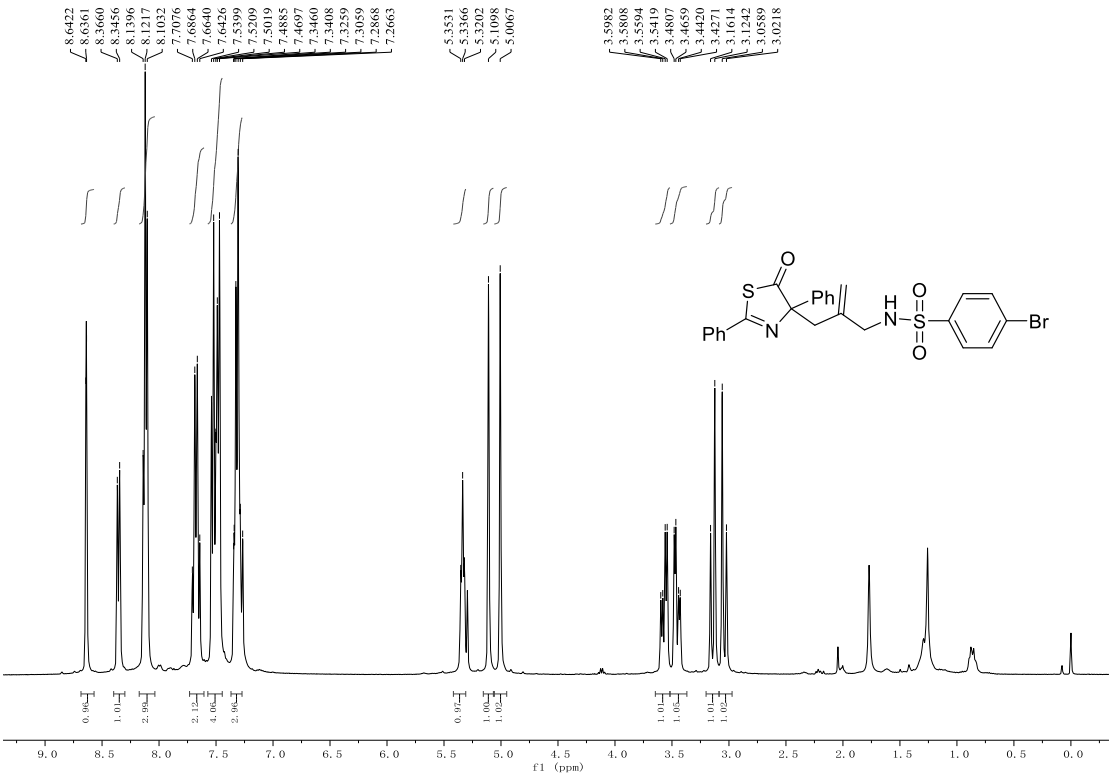


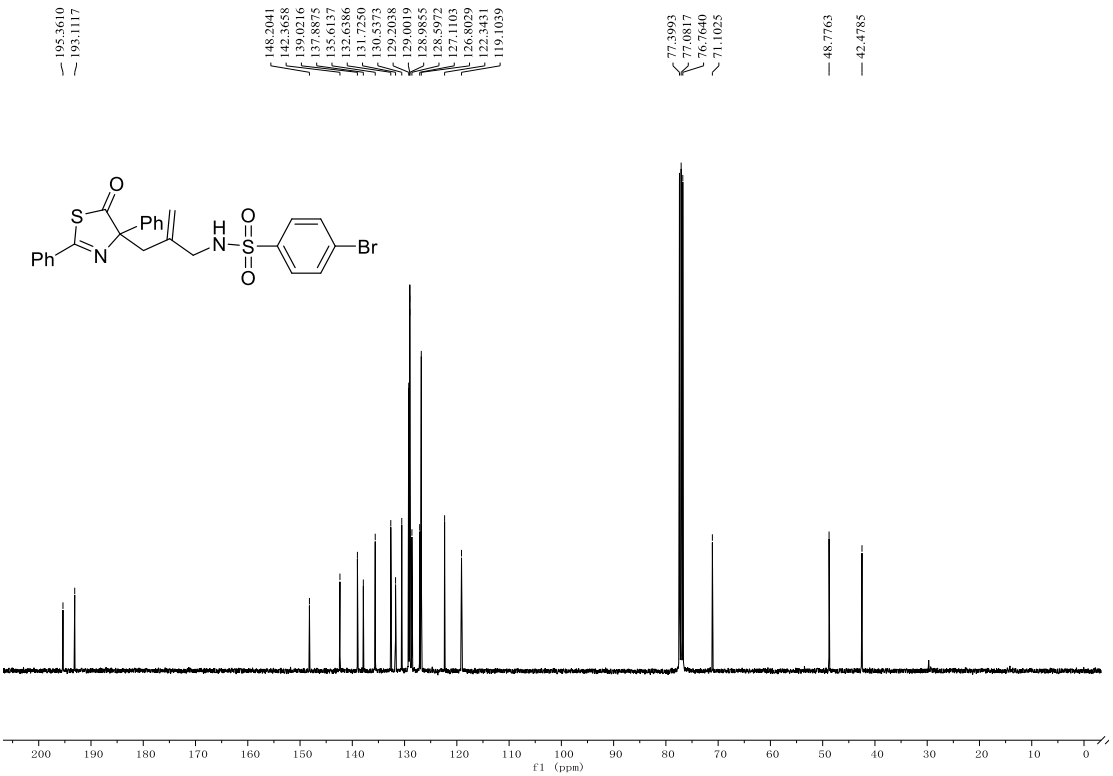
^{1}H and ^{13}C NMR spectra for compound 3j



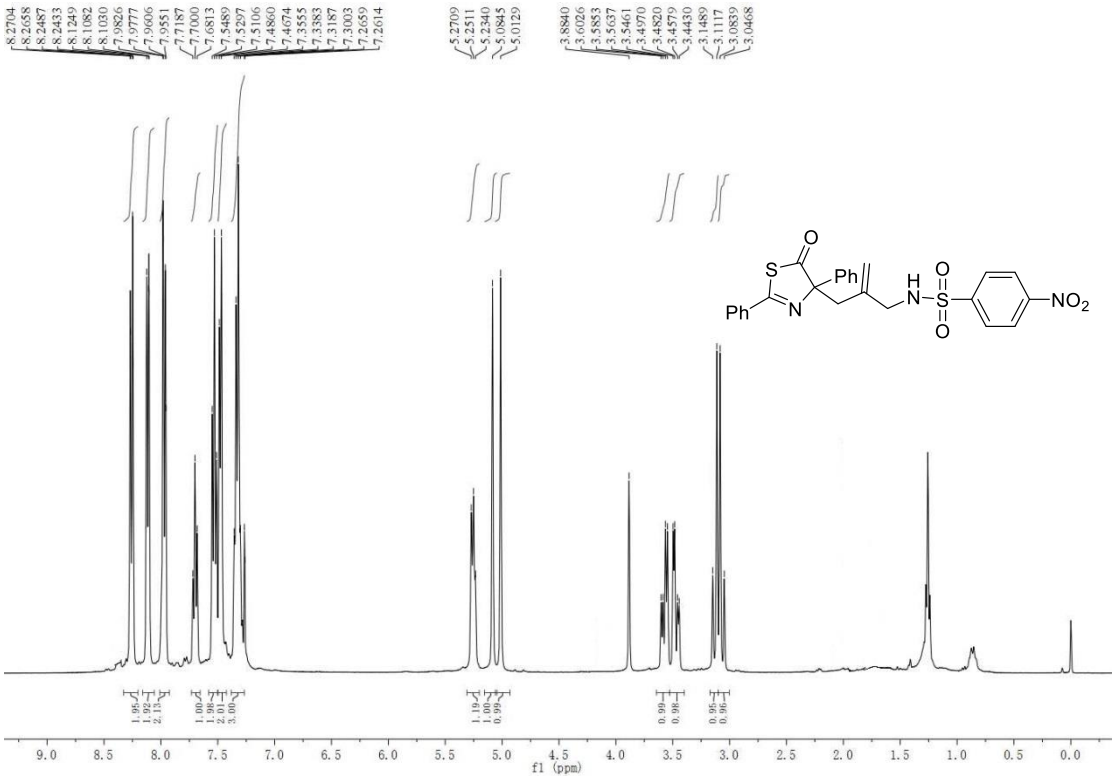


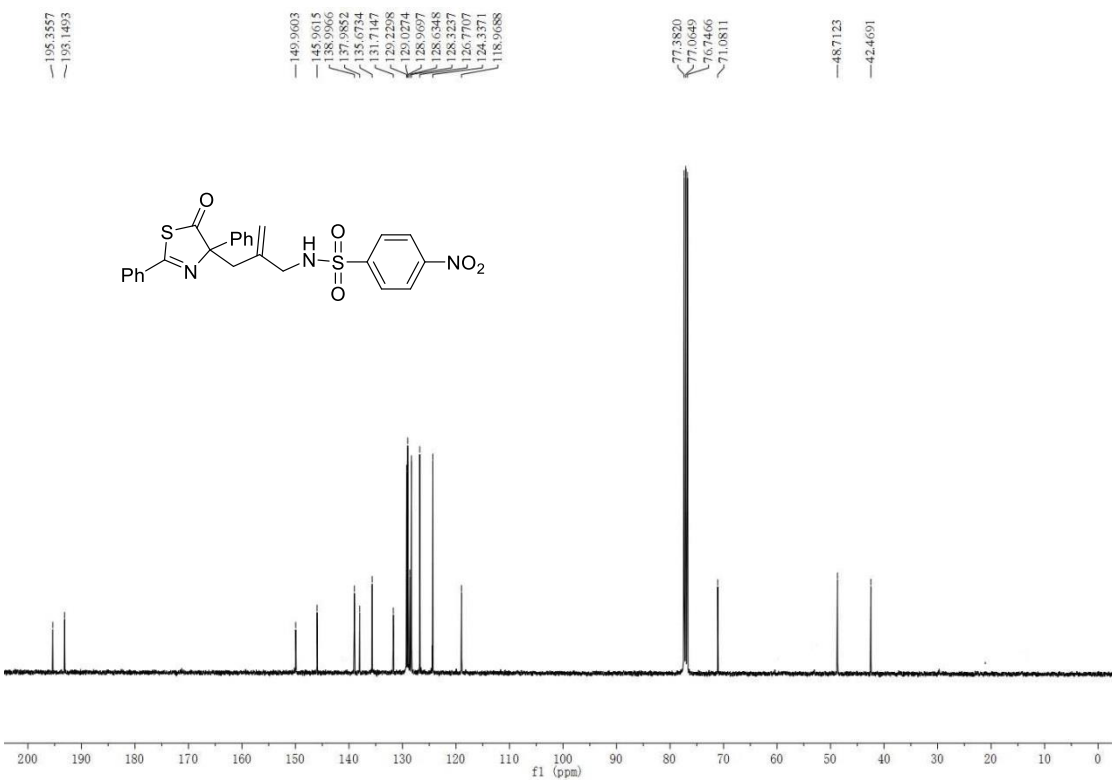
^{1}H and ^{13}C NMR spectra for compound 3k



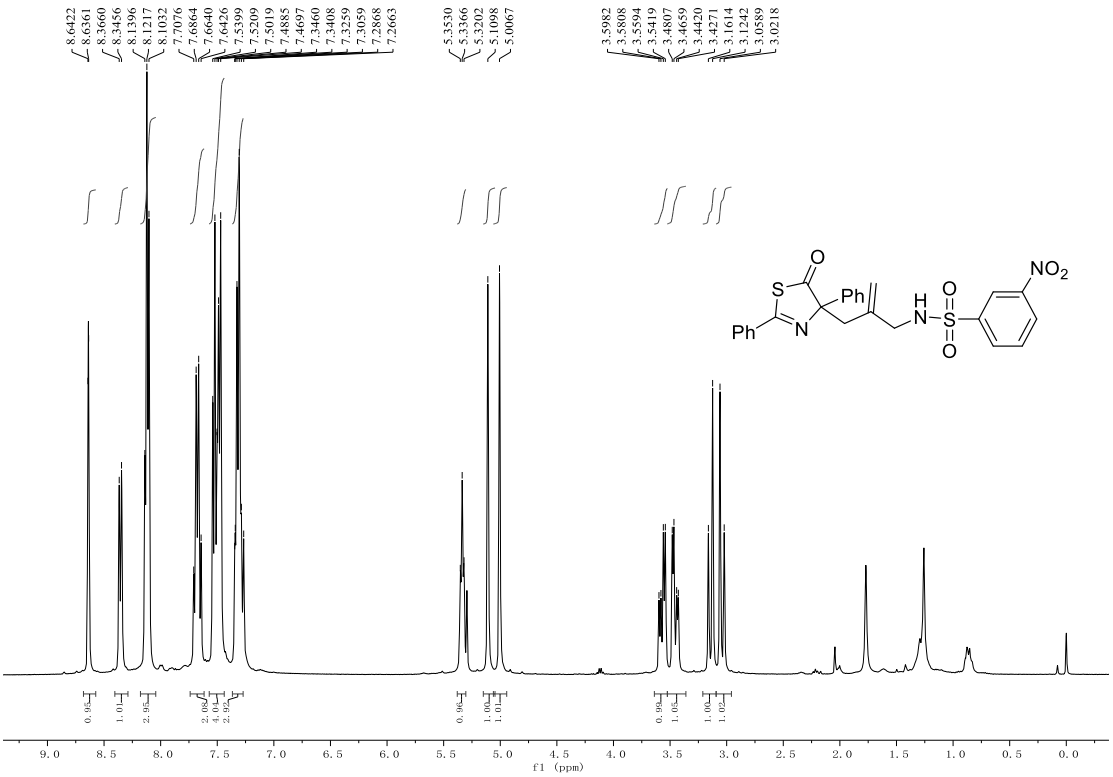


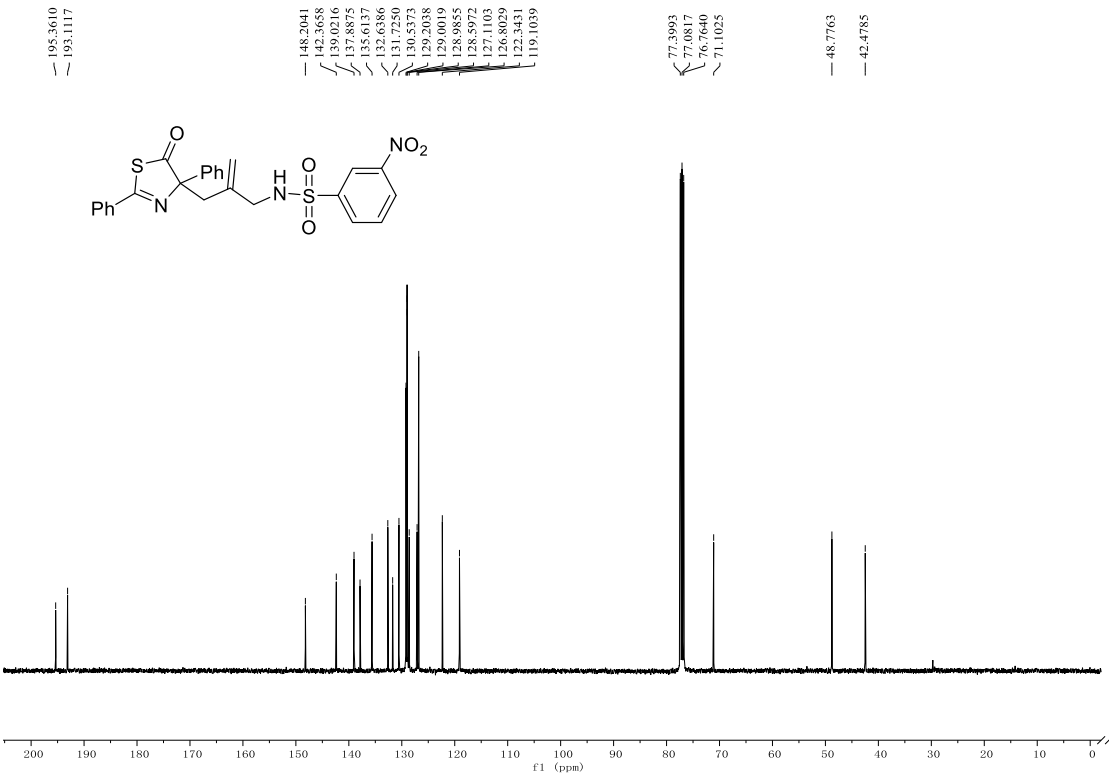
^{1}H and ^{13}C NMR spectra for compound 3l



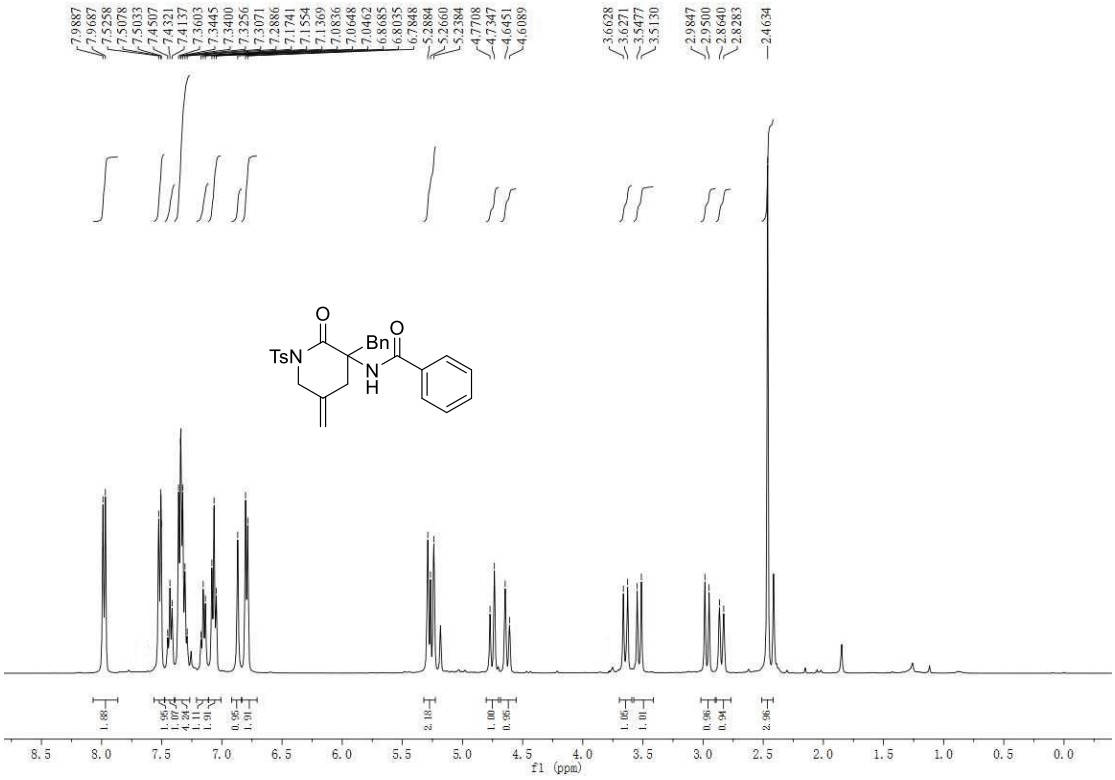


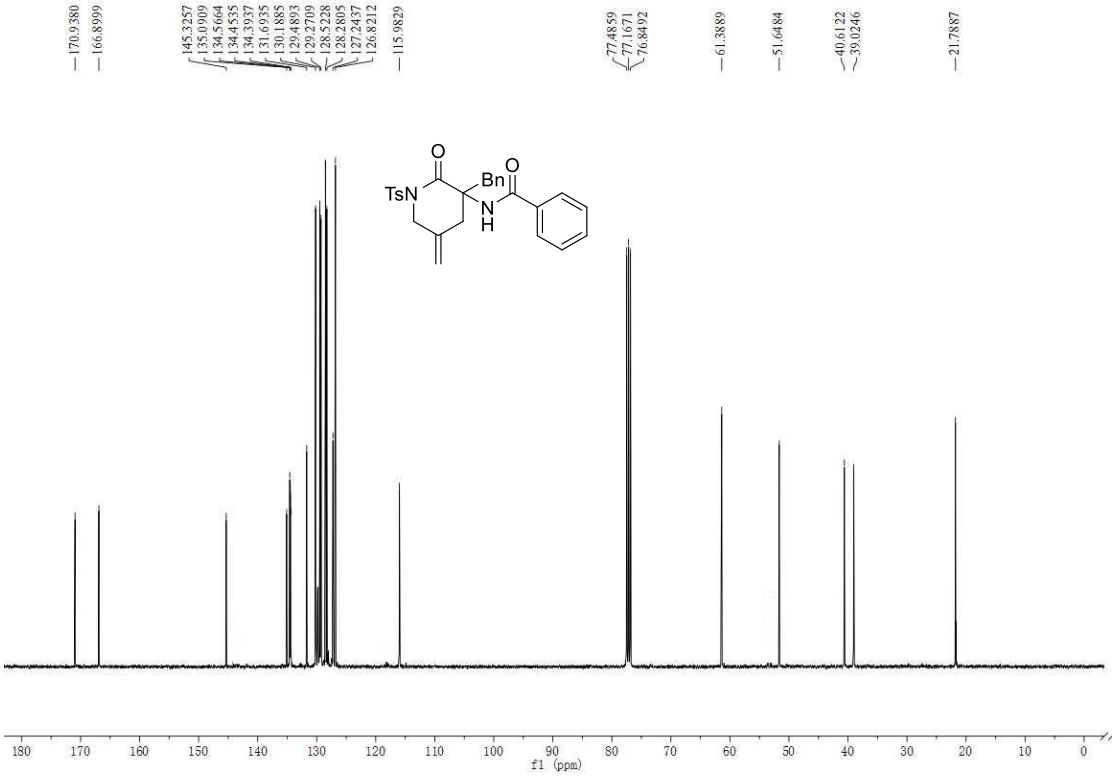
^{1}H and ^{13}C NMR spectra for compound 3m



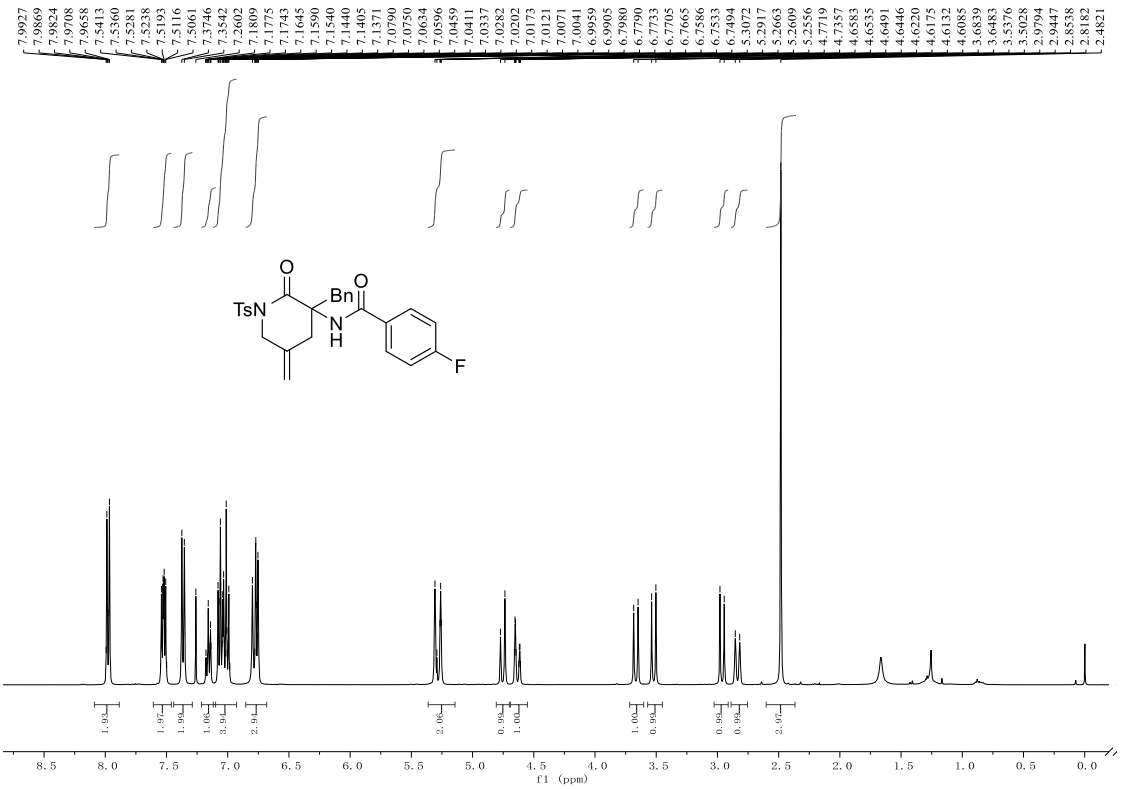


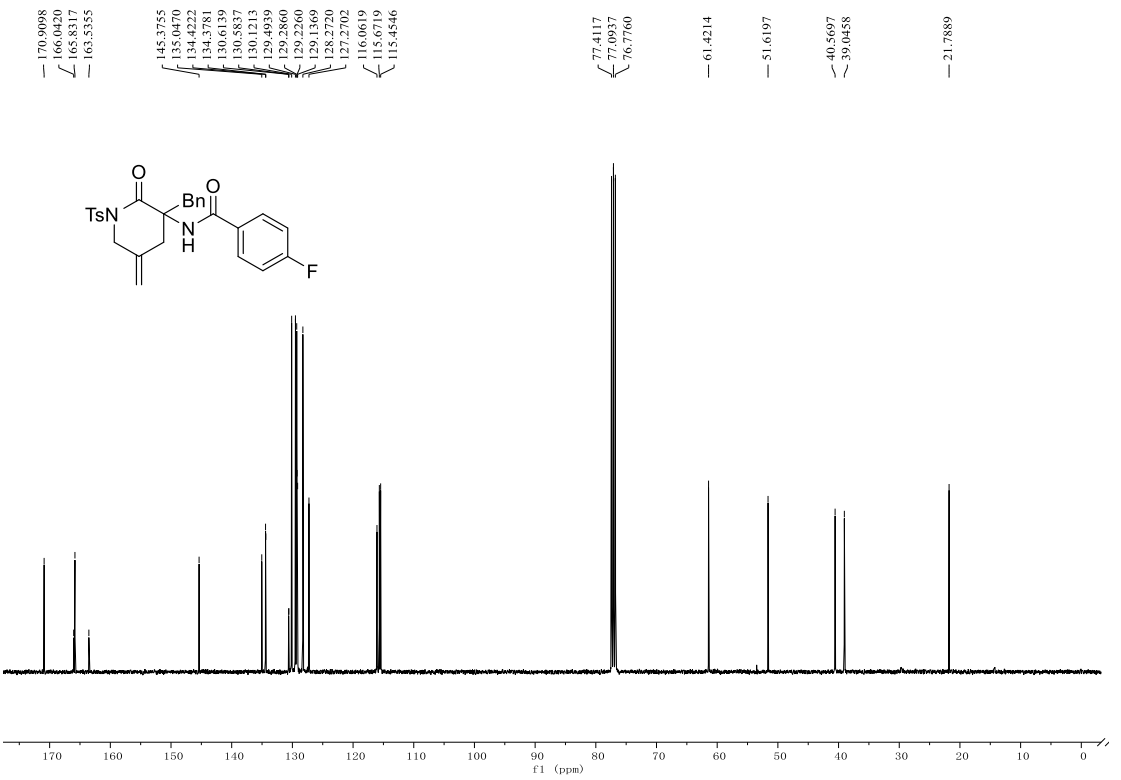
^{1}H and ^{13}C NMR spectra for compound 5a



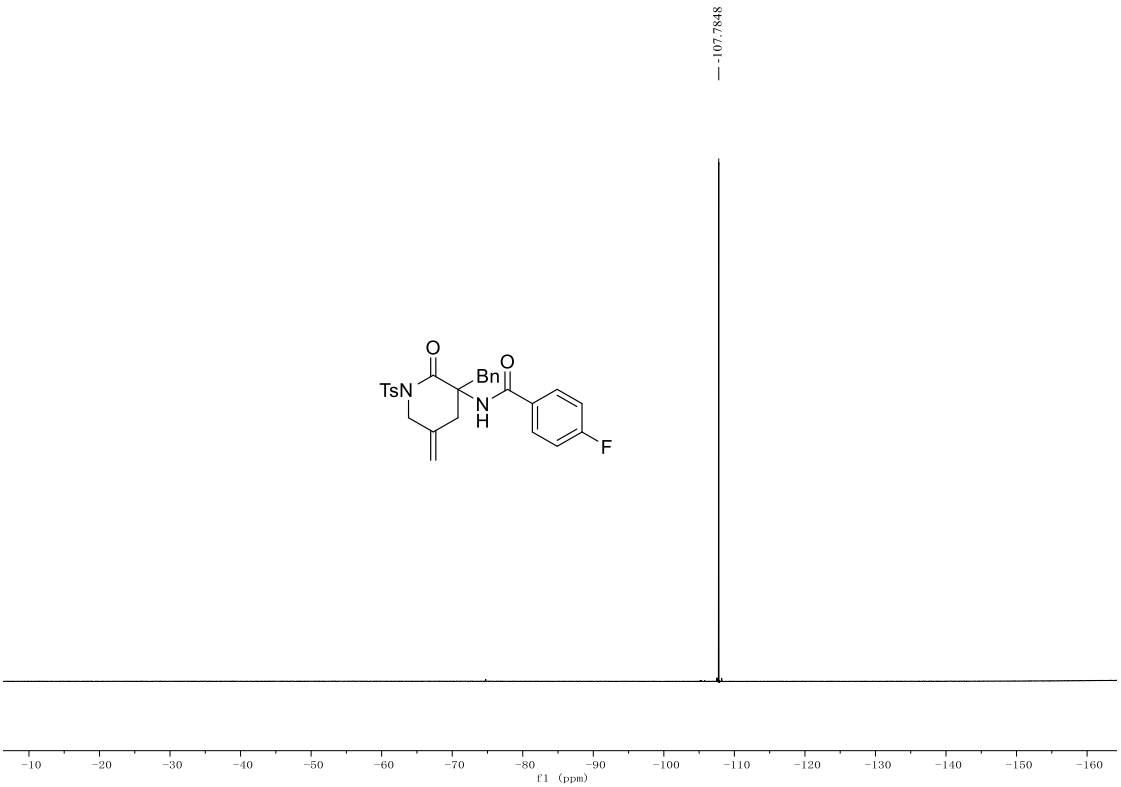


^{1}H and ^{13}C NMR spectra for compound 5b

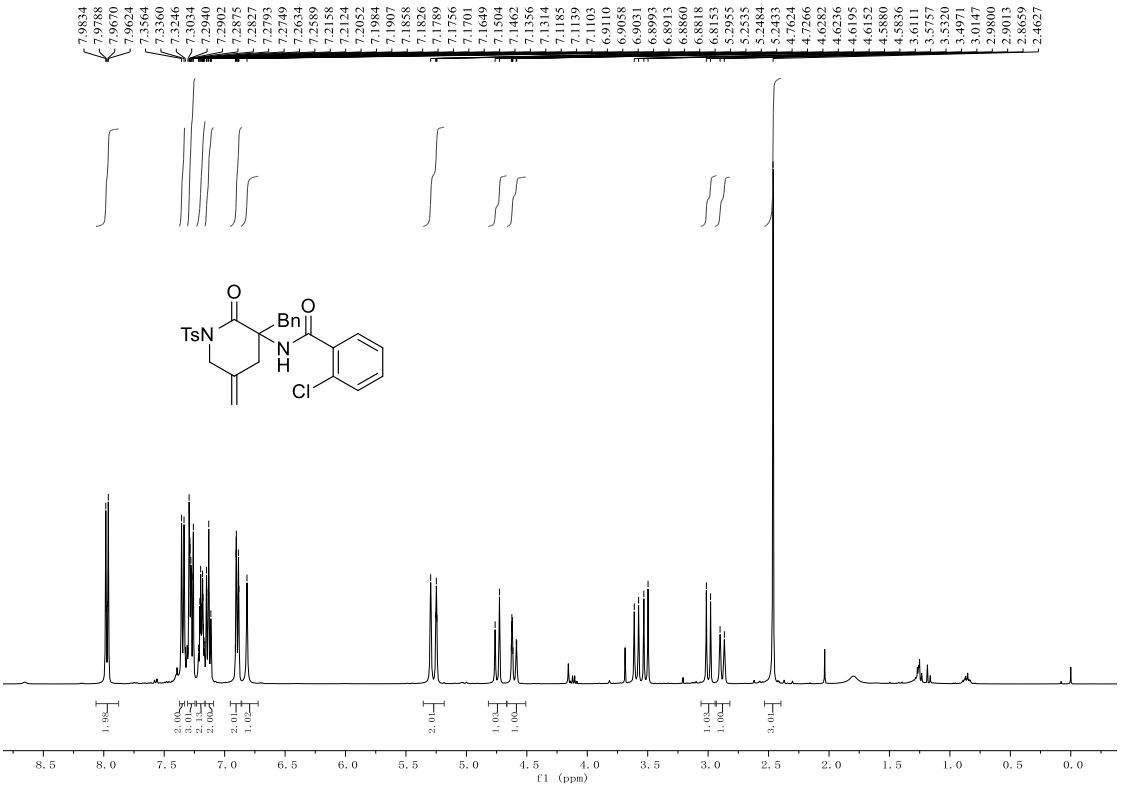


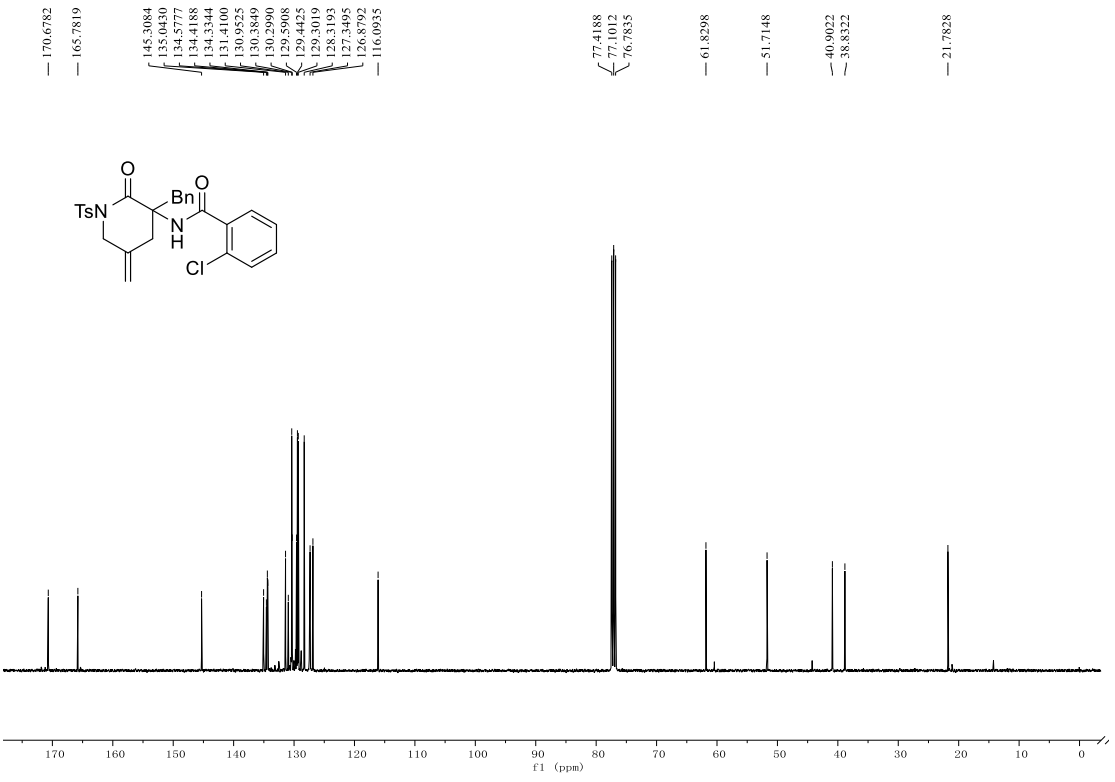


^{19}F NMR spectra for compound 5b

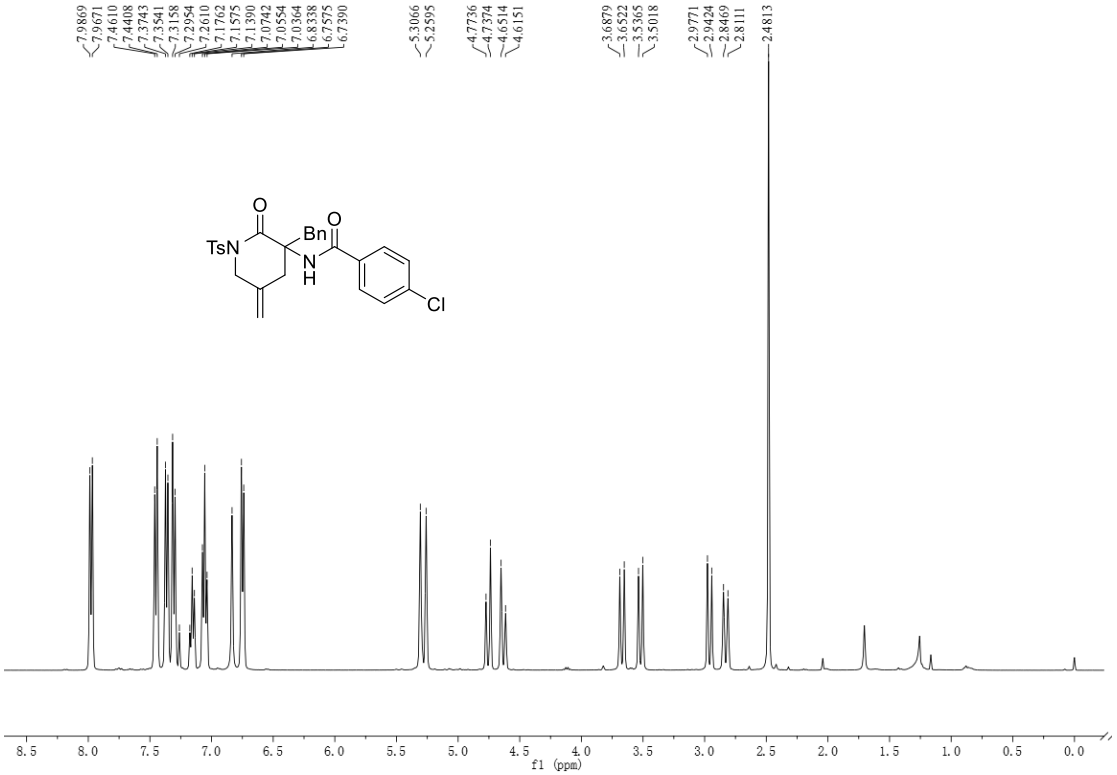


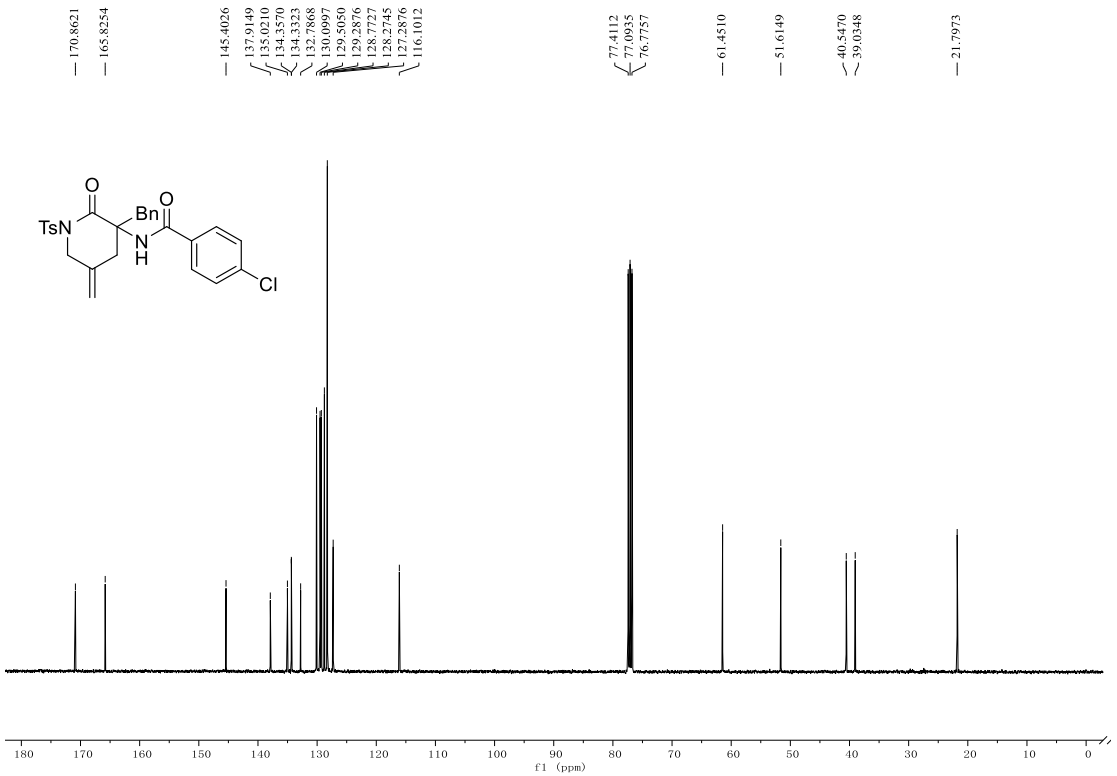
^{1}H and ^{13}C NMR spectra for compound 5c



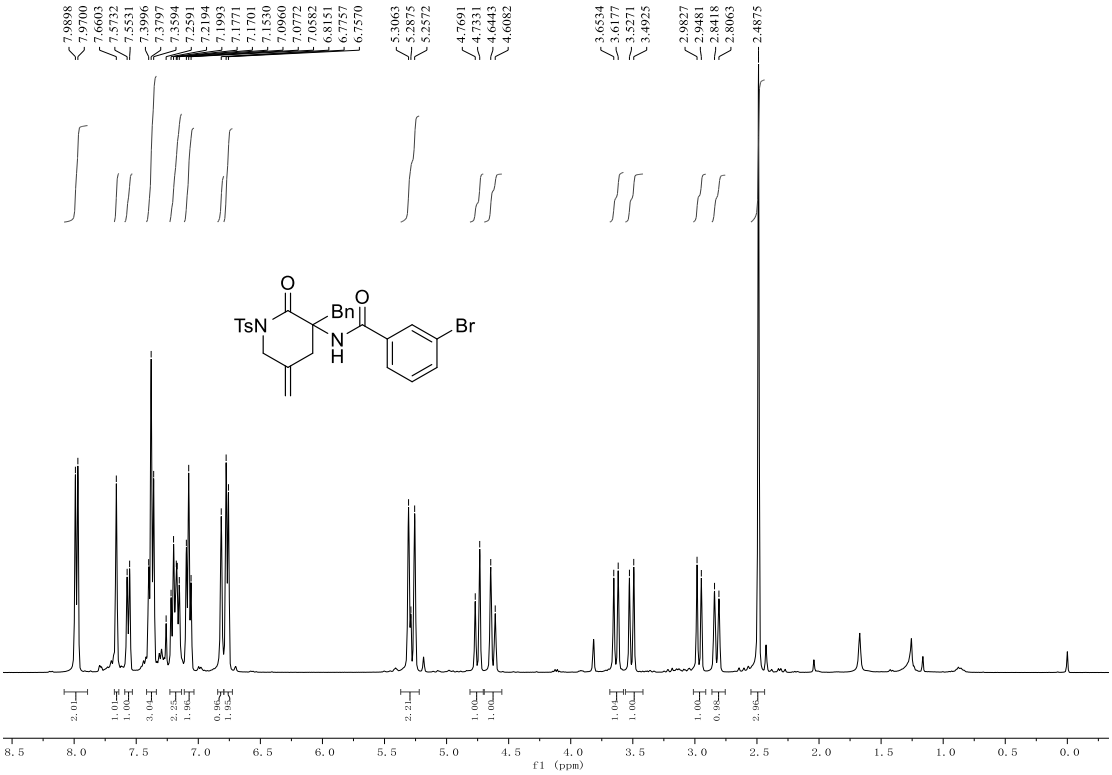


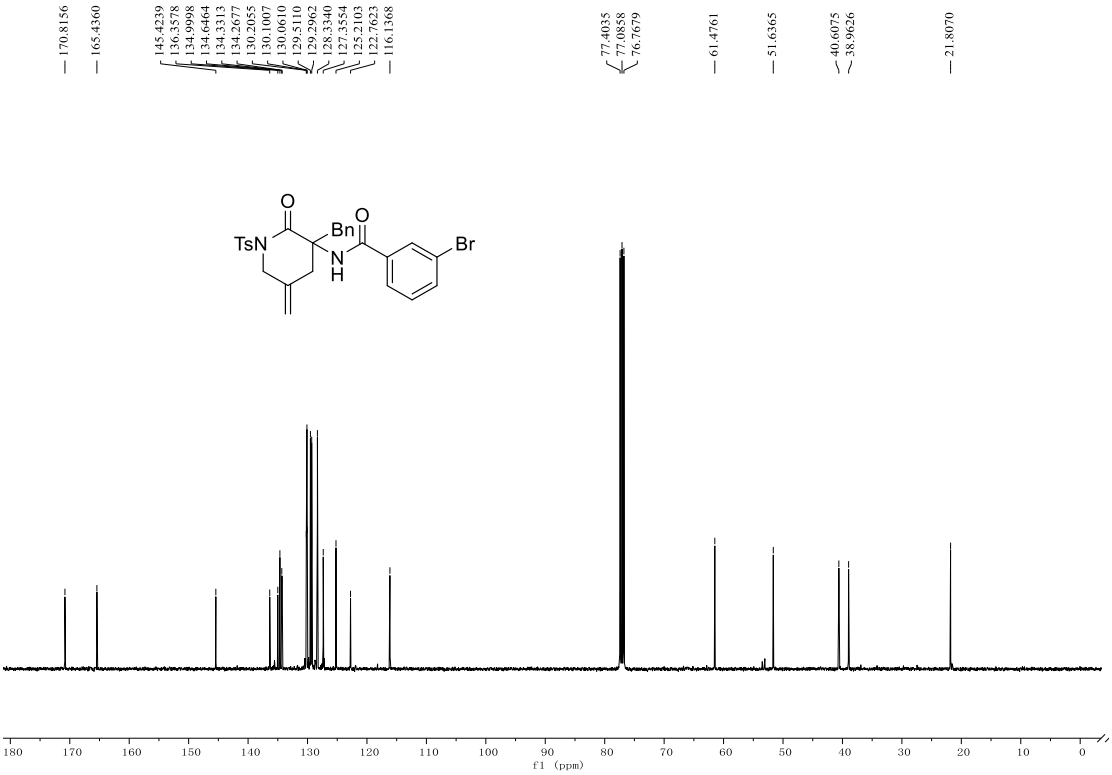
^{1}H and ^{13}C NMR spectra for compound 5d



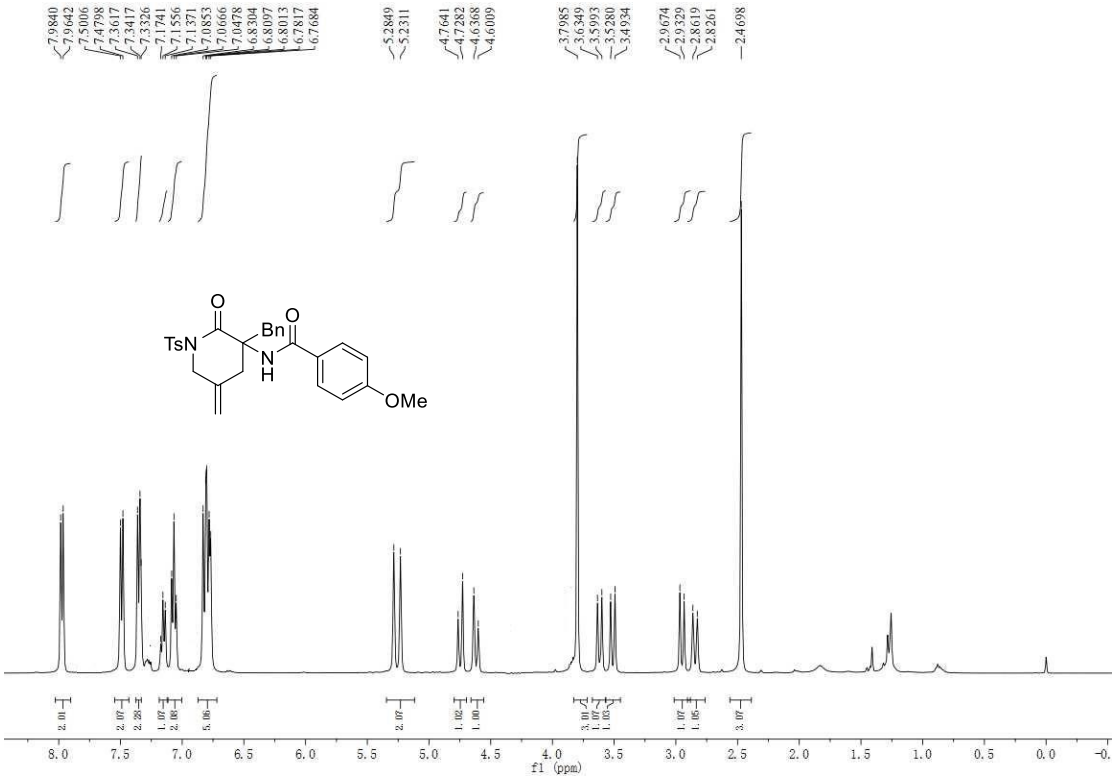


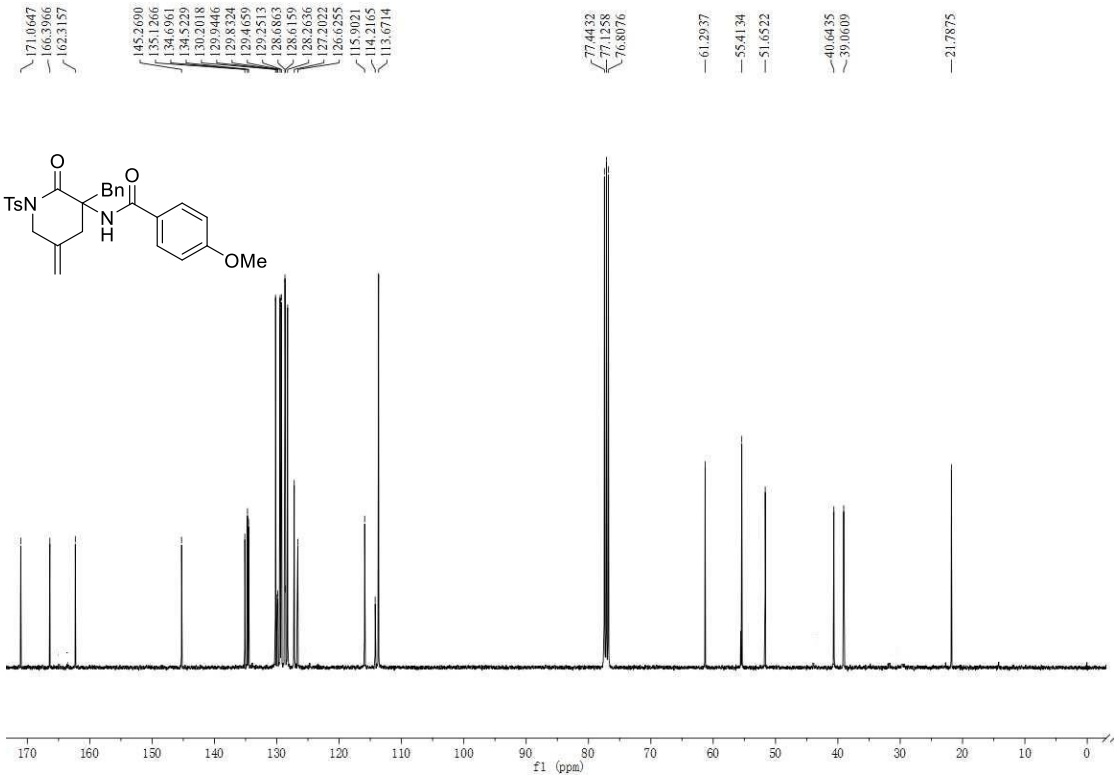
^{1}H and ^{13}C NMR spectra for compound 5e



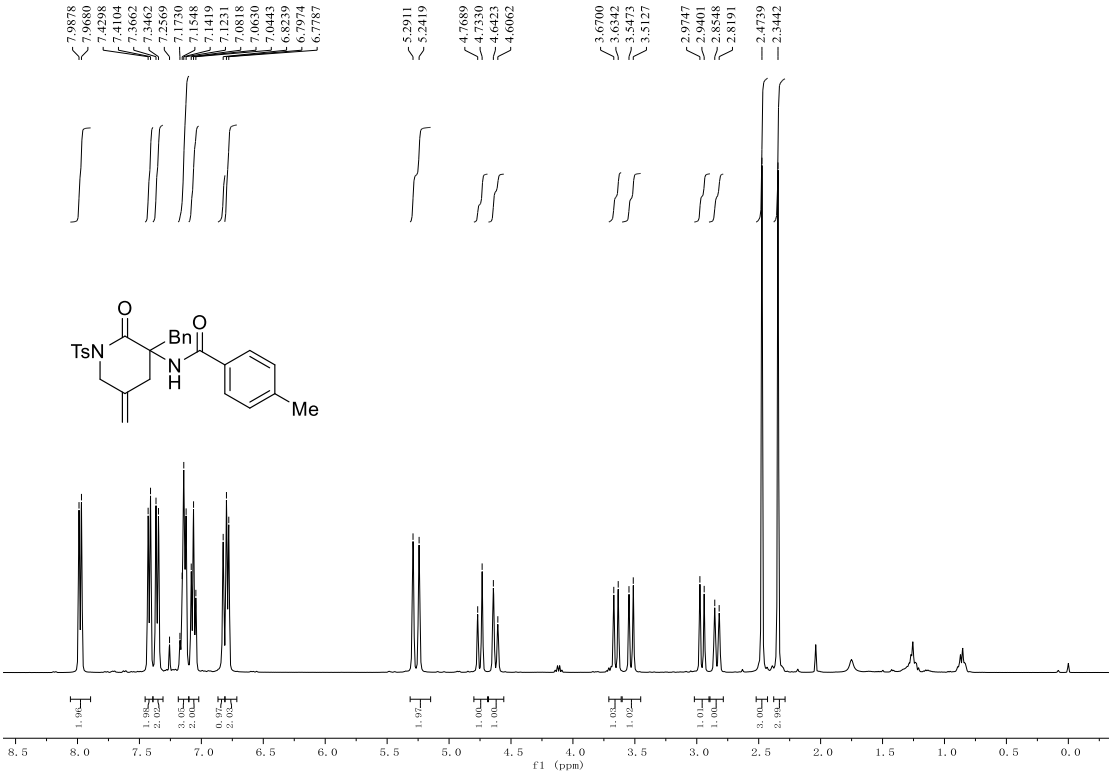


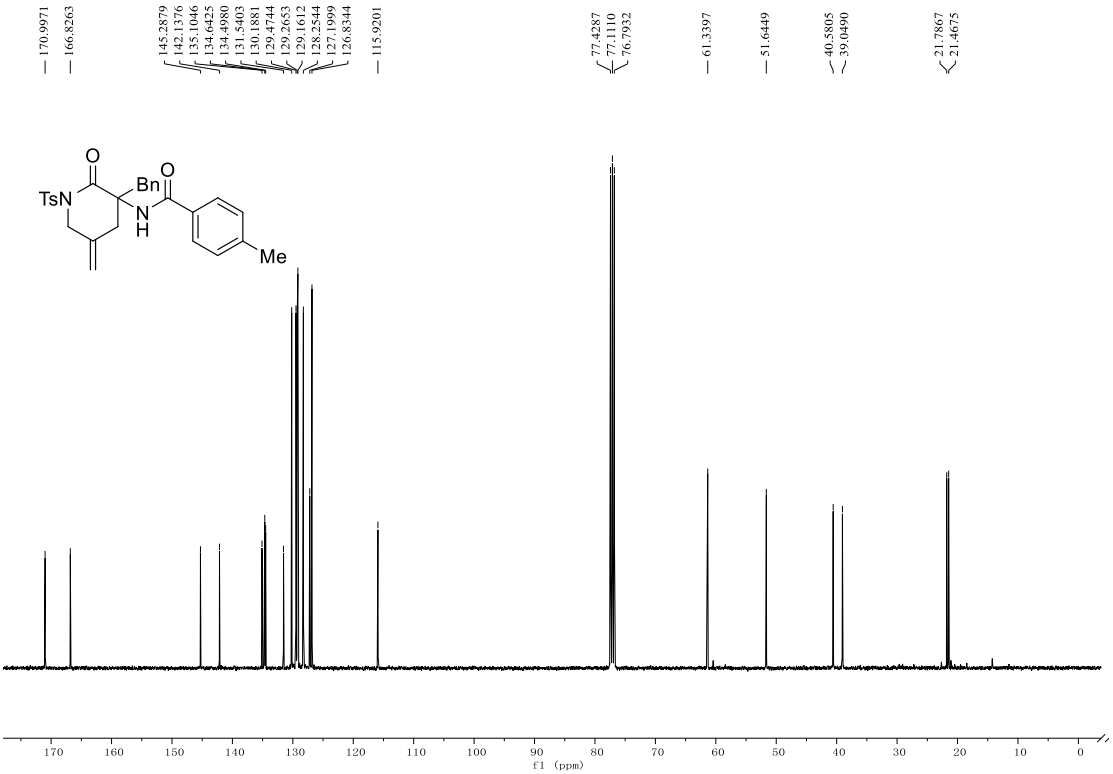
^{1}H and ^{13}C NMR spectra for compound 5f



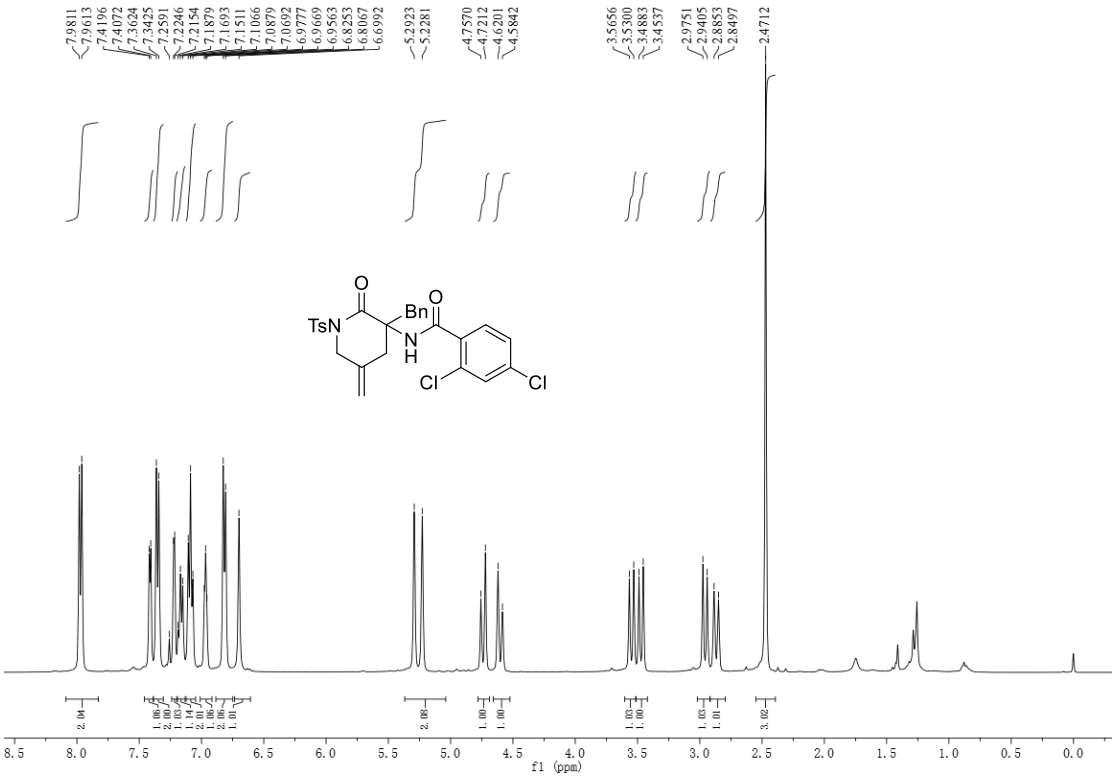


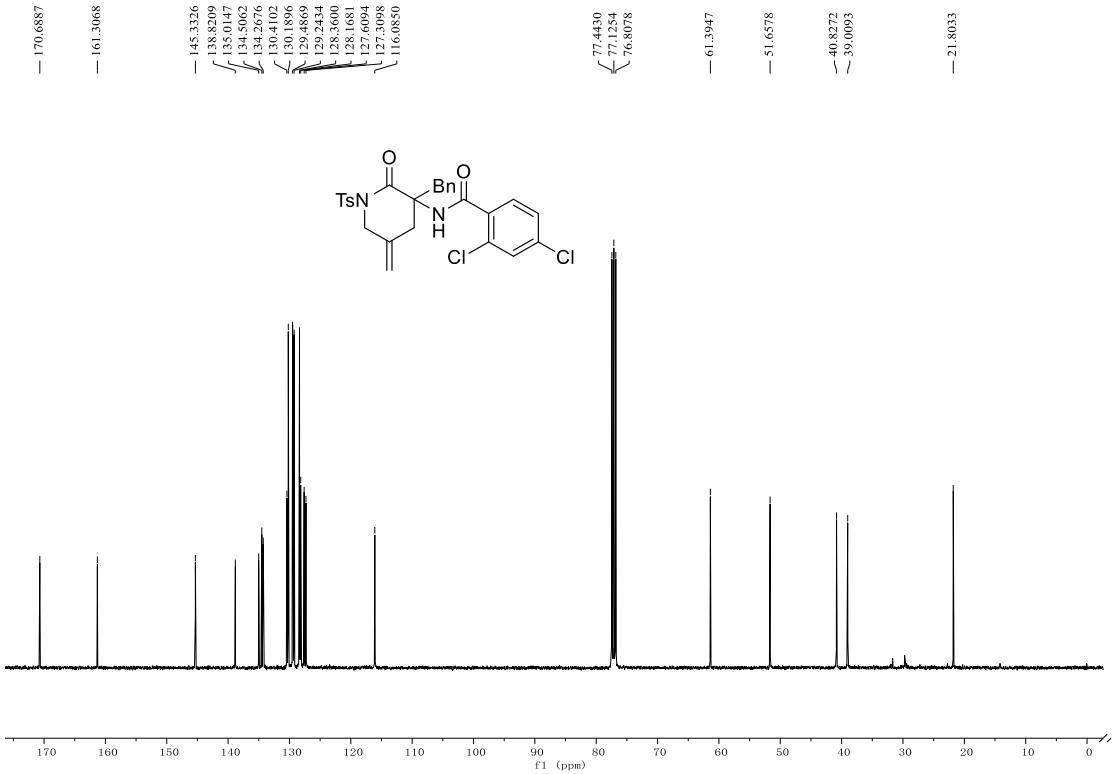
^{1}H and ^{13}C NMR spectra for compound 5g



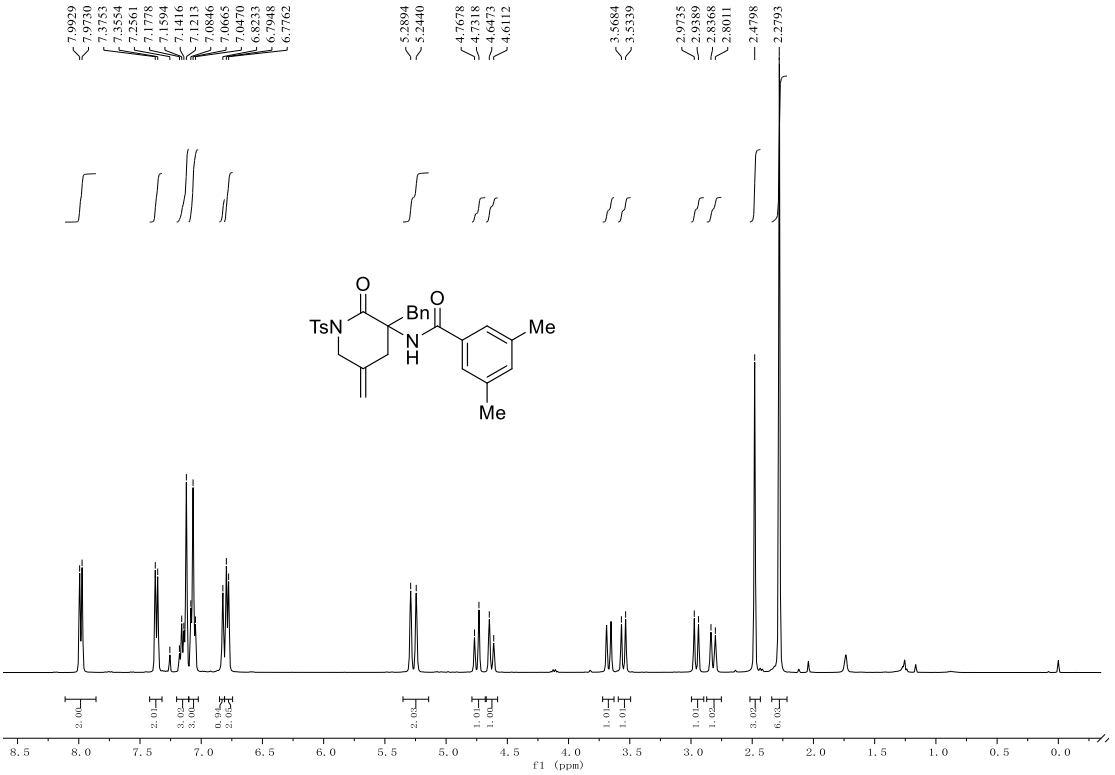


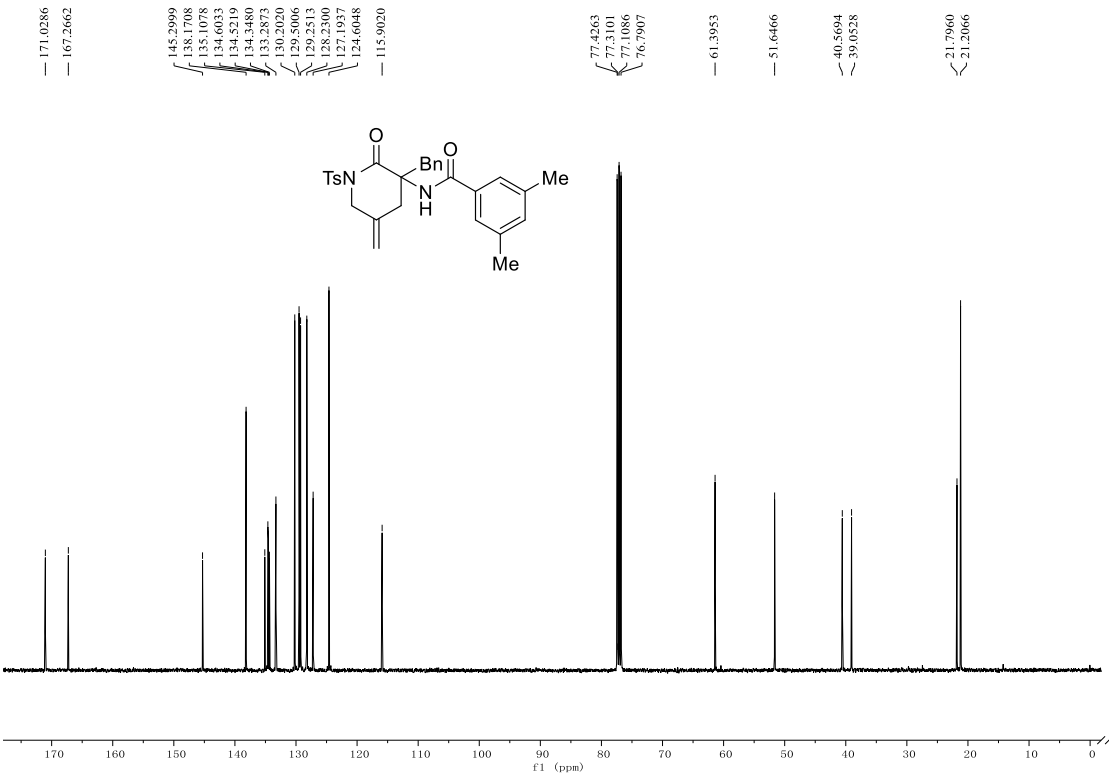
^{1}H and ^{13}C NMR spectra for compound 5h



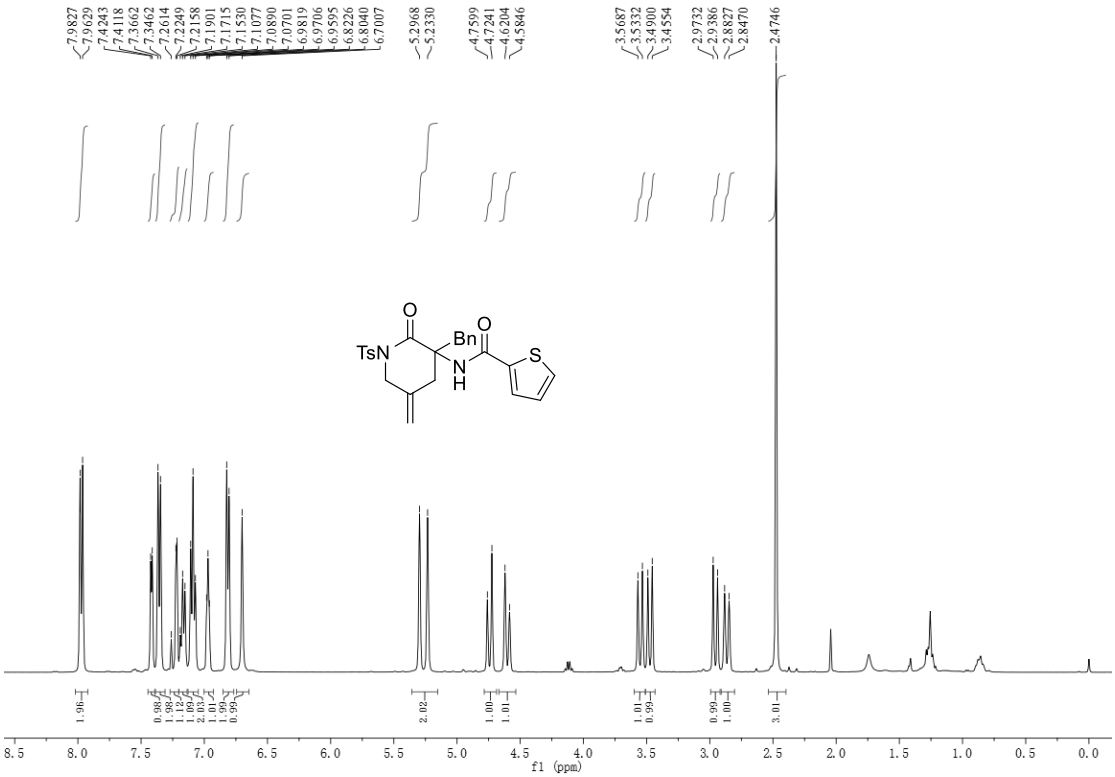


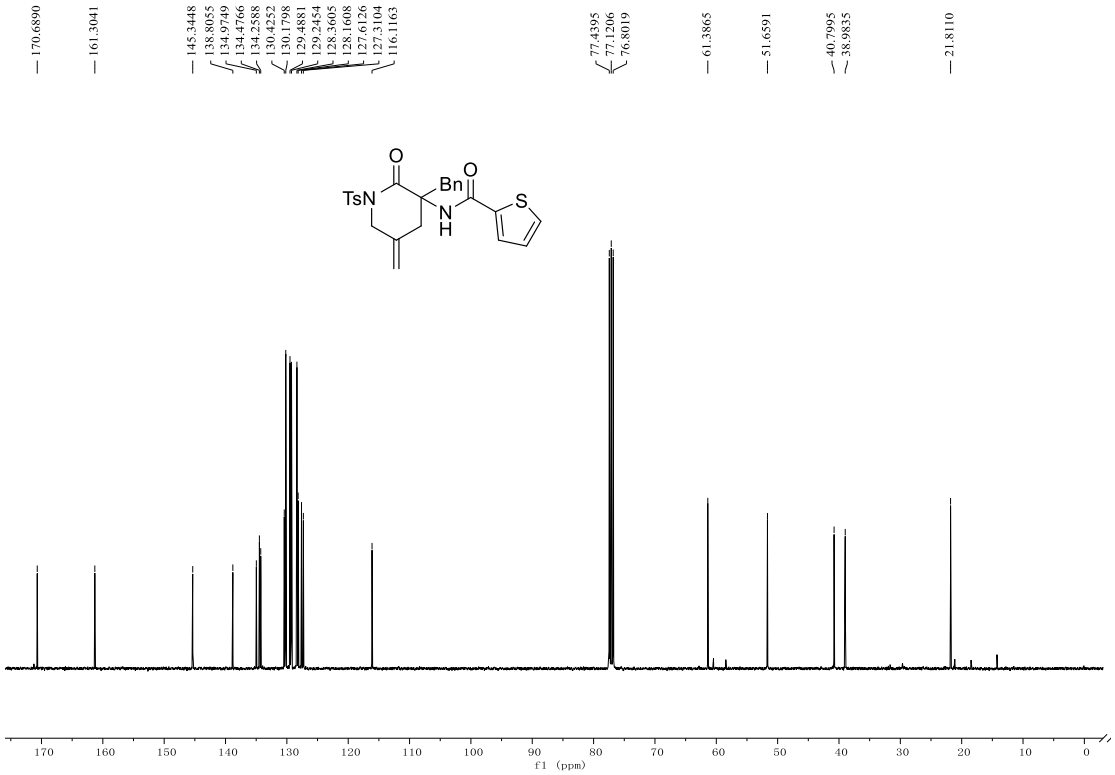
^{1}H and ^{13}C NMR spectra for compound 5i



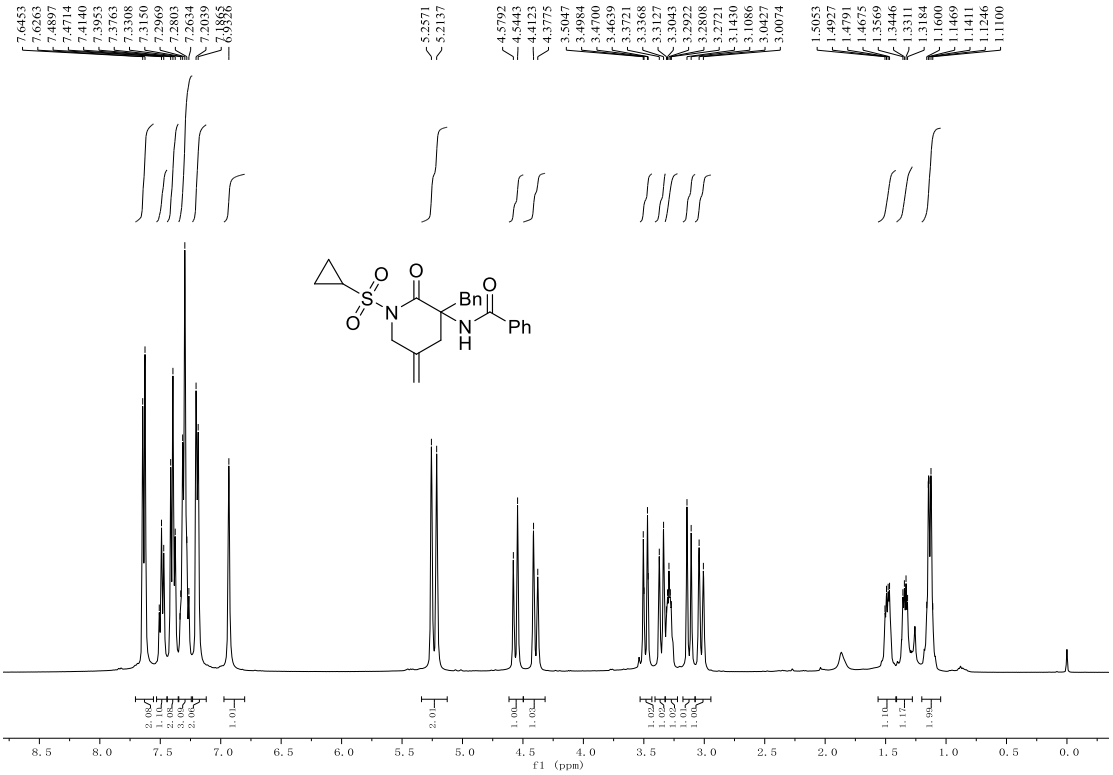


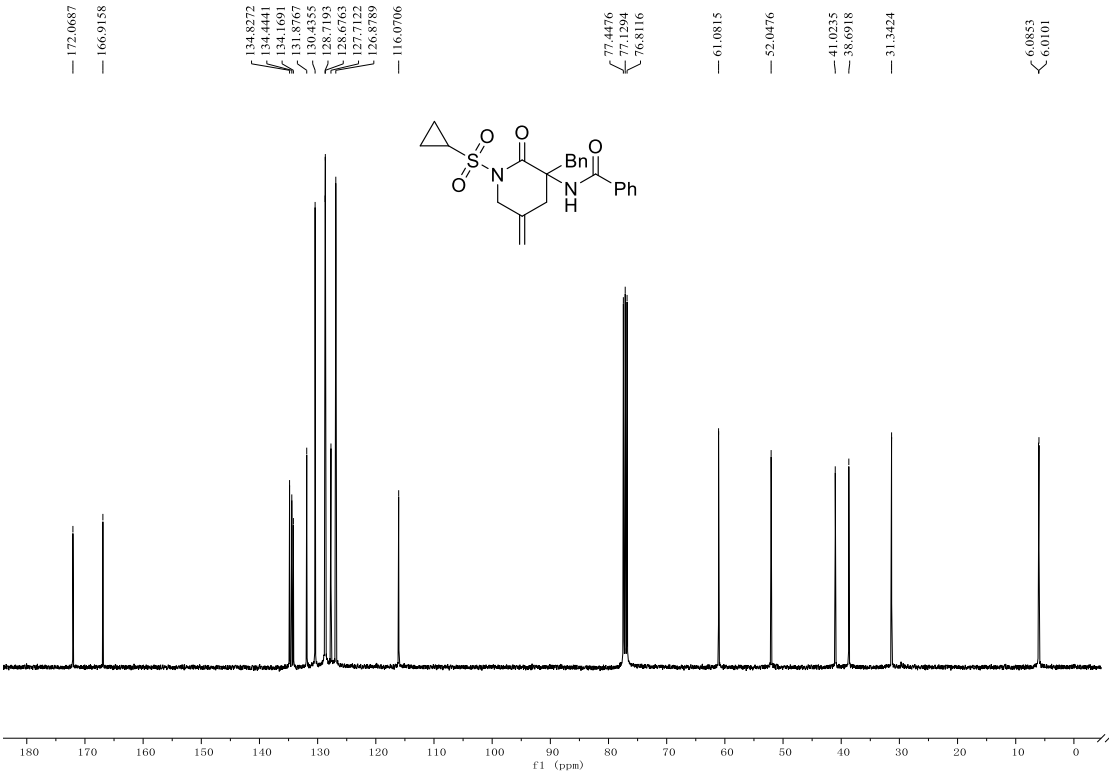
^{1}H and ^{13}C NMR spectra for compound 5j



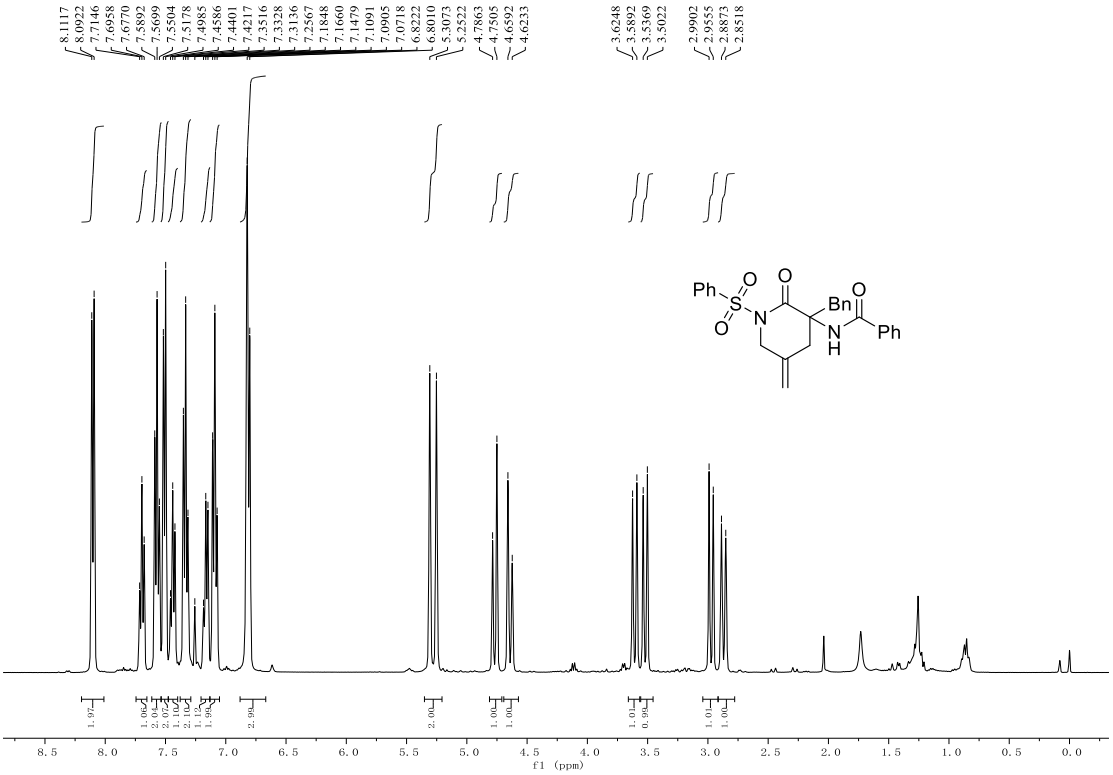


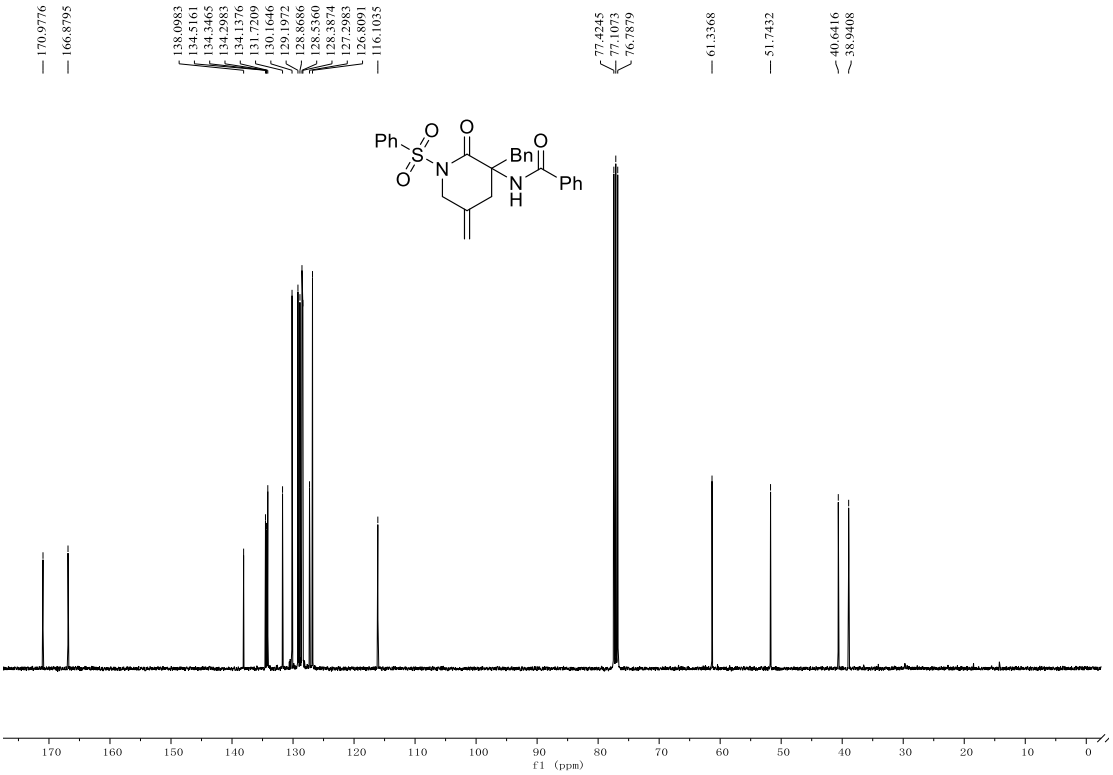
^{1}H and ^{13}C NMR spectra for compound 5k



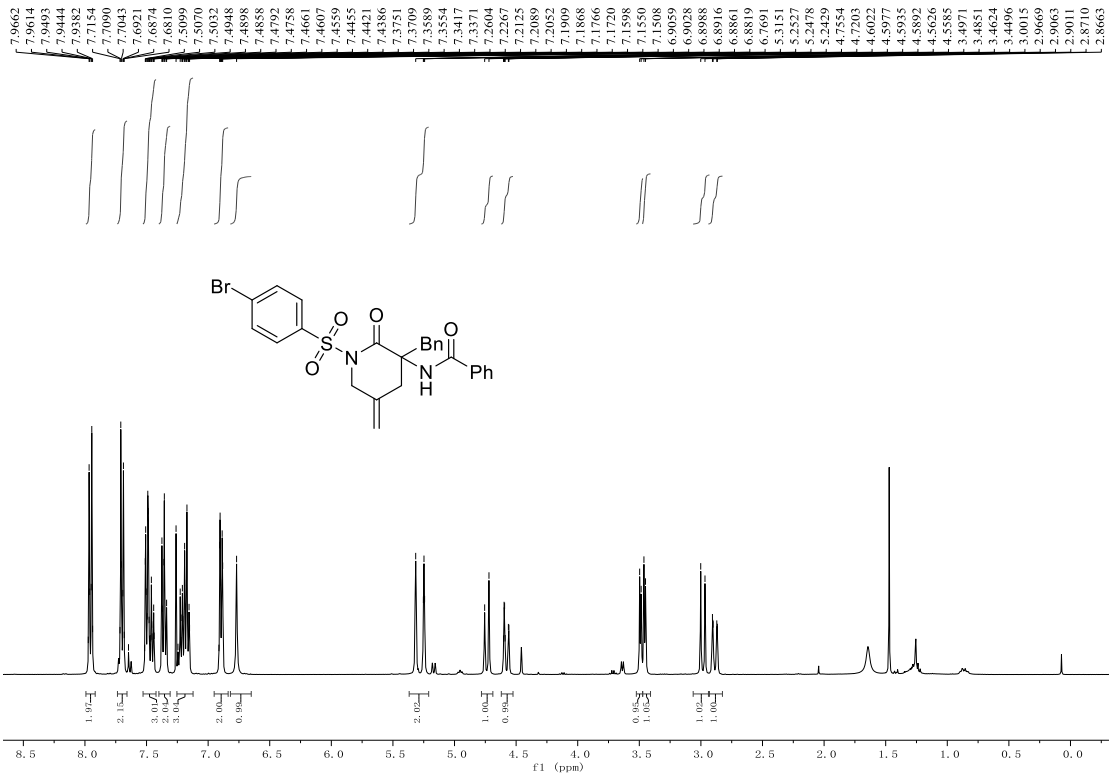


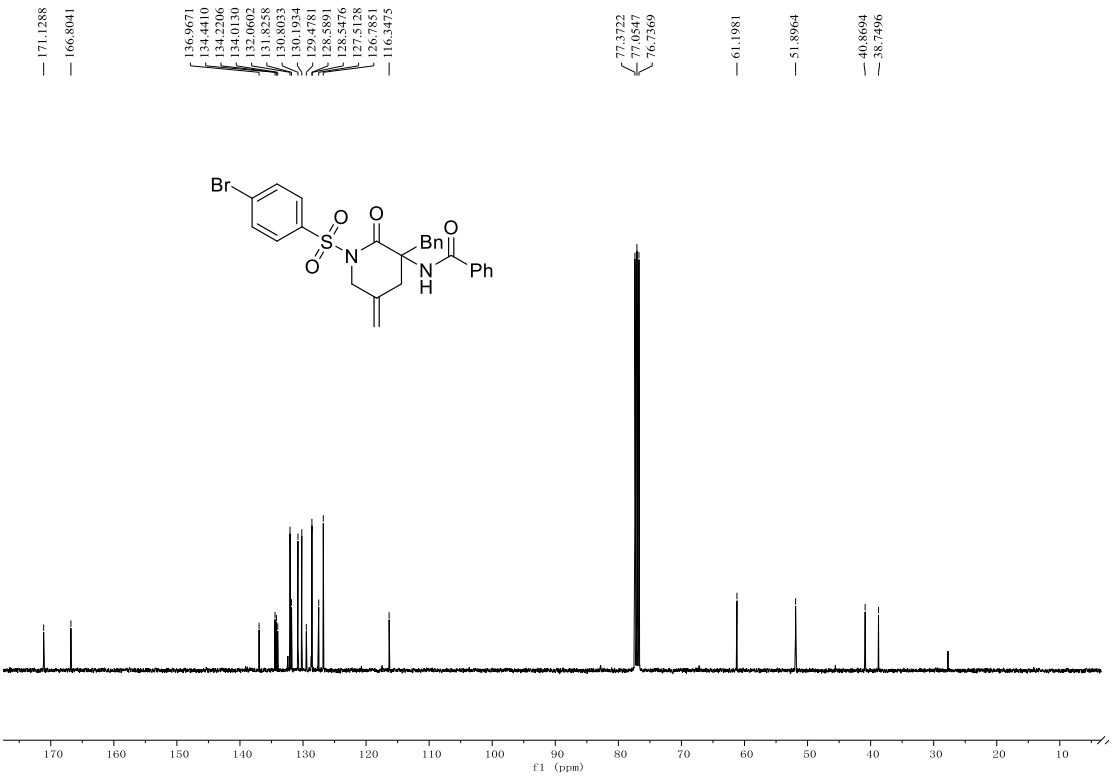
^{1}H and ^{13}C NMR spectra for compound 5l



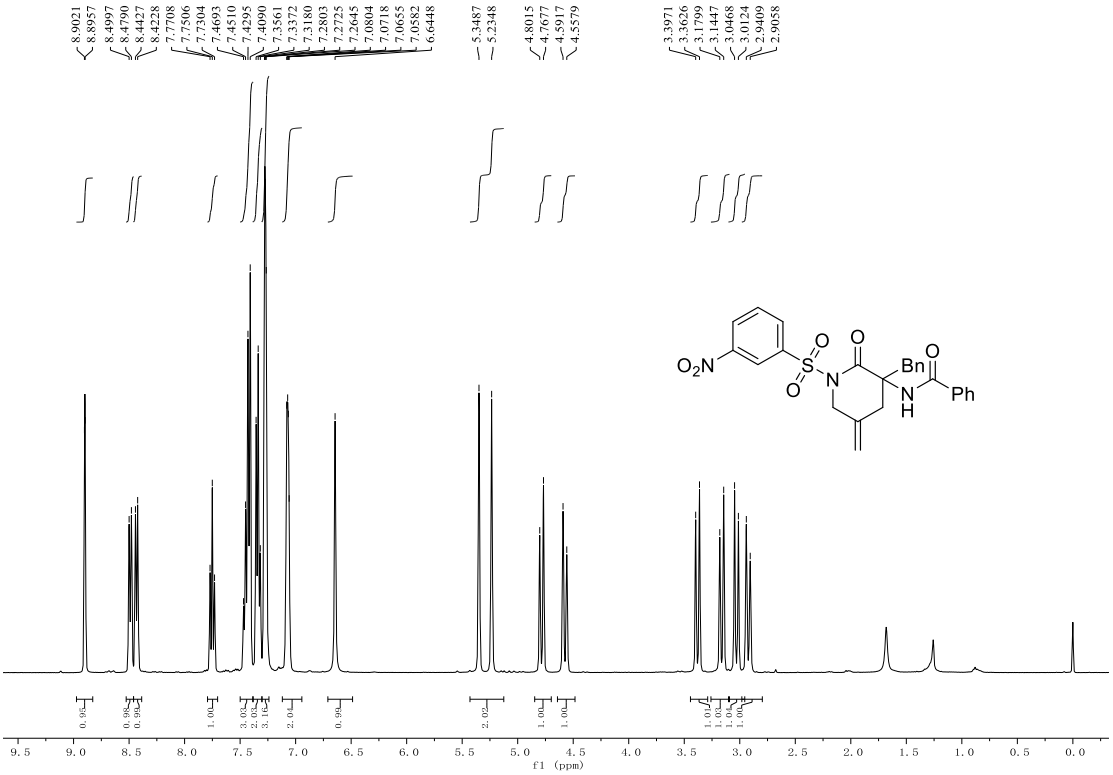


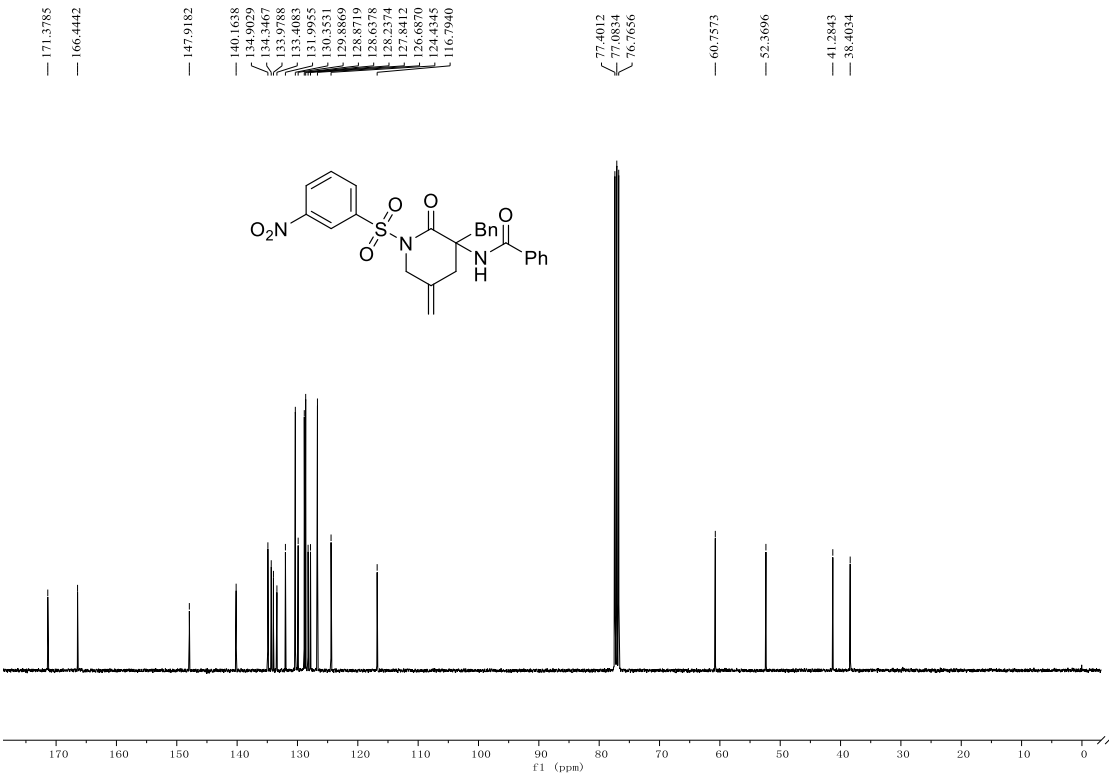
^{1}H and ^{13}C NMR spectra for compound 5m





^{1}H and ^{13}C NMR spectra for compound 5n





^{1}H and ^{13}C NMR spectra for compound 6