

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

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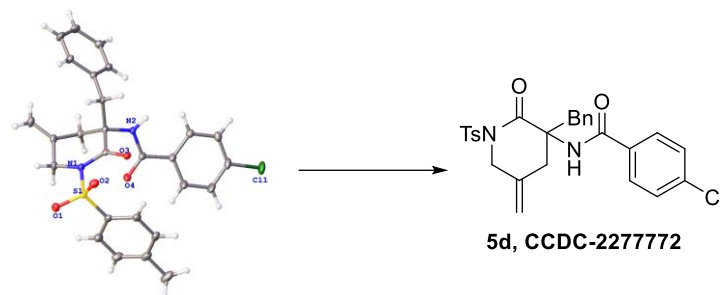
Supporting Information

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1. X-Ray crystal data for compound **5d**

Single crystal of compound **5d** was prepared from the mixture solvent of EtOH and CH₂Cl₂. 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.



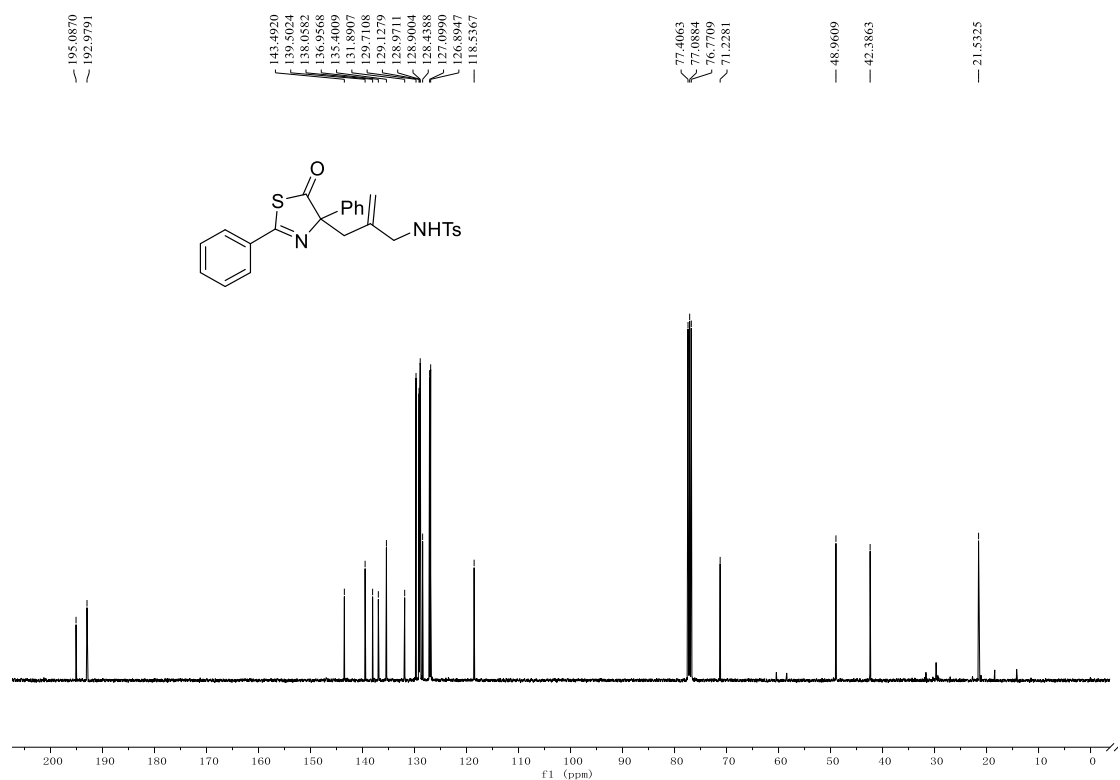
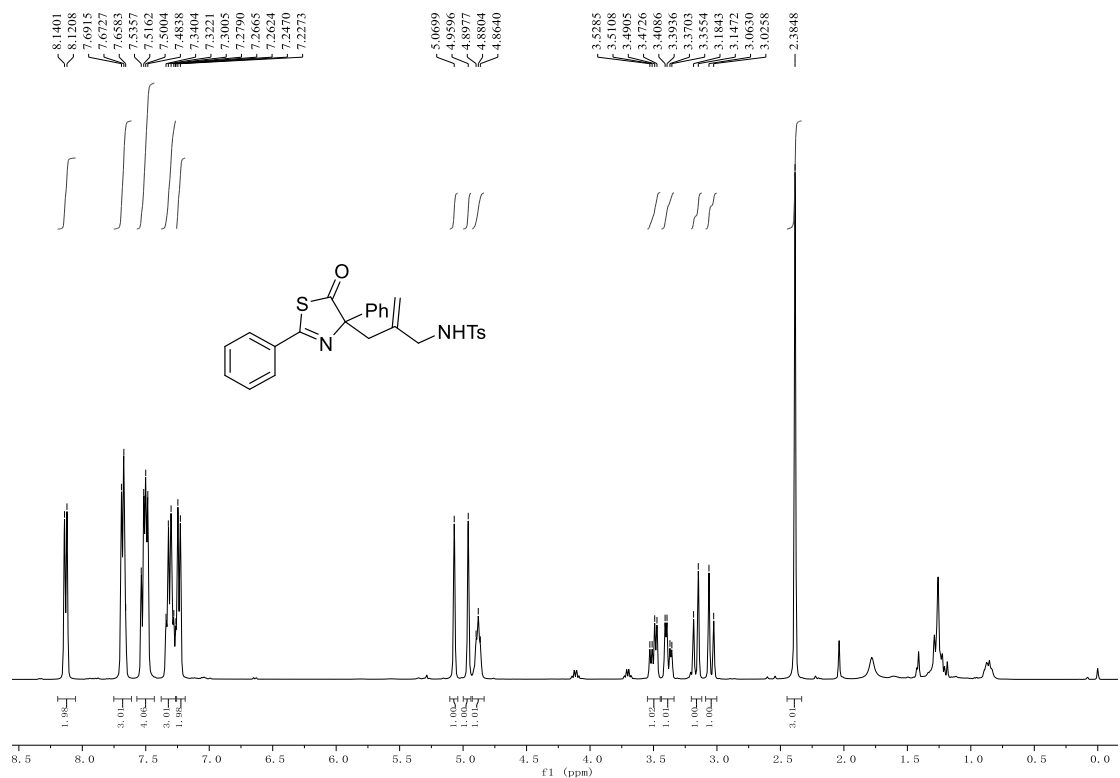
ORTEP of **5d** (at 50% level)

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

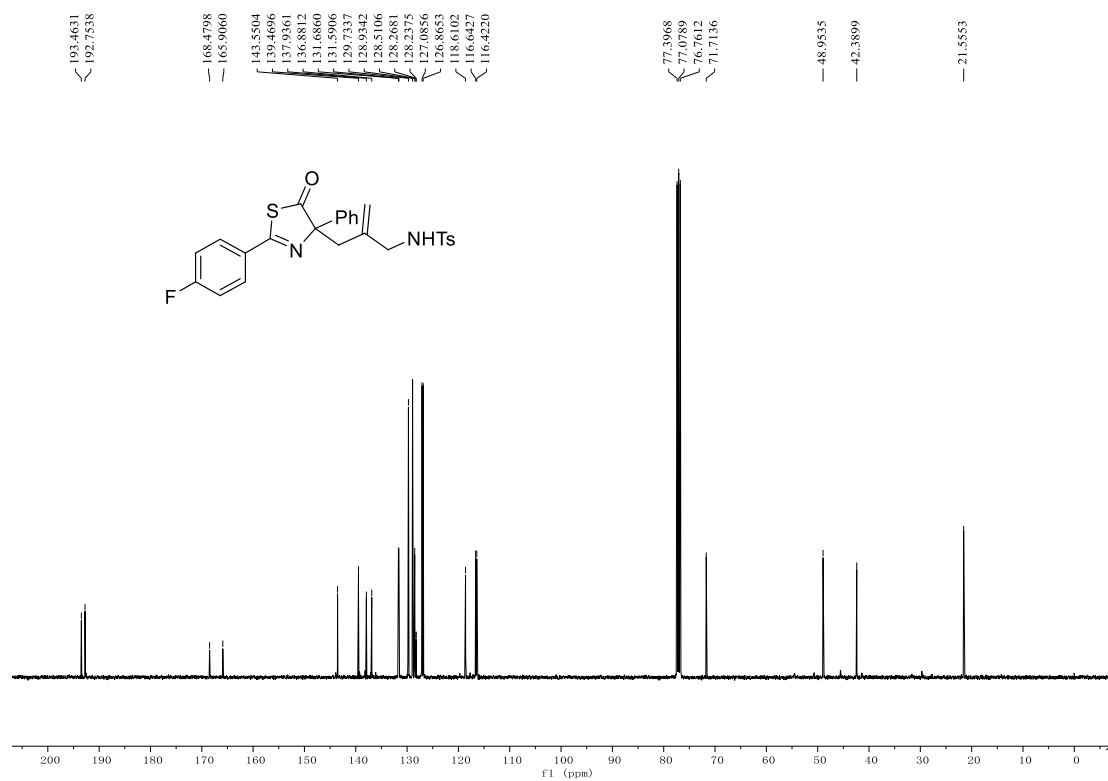
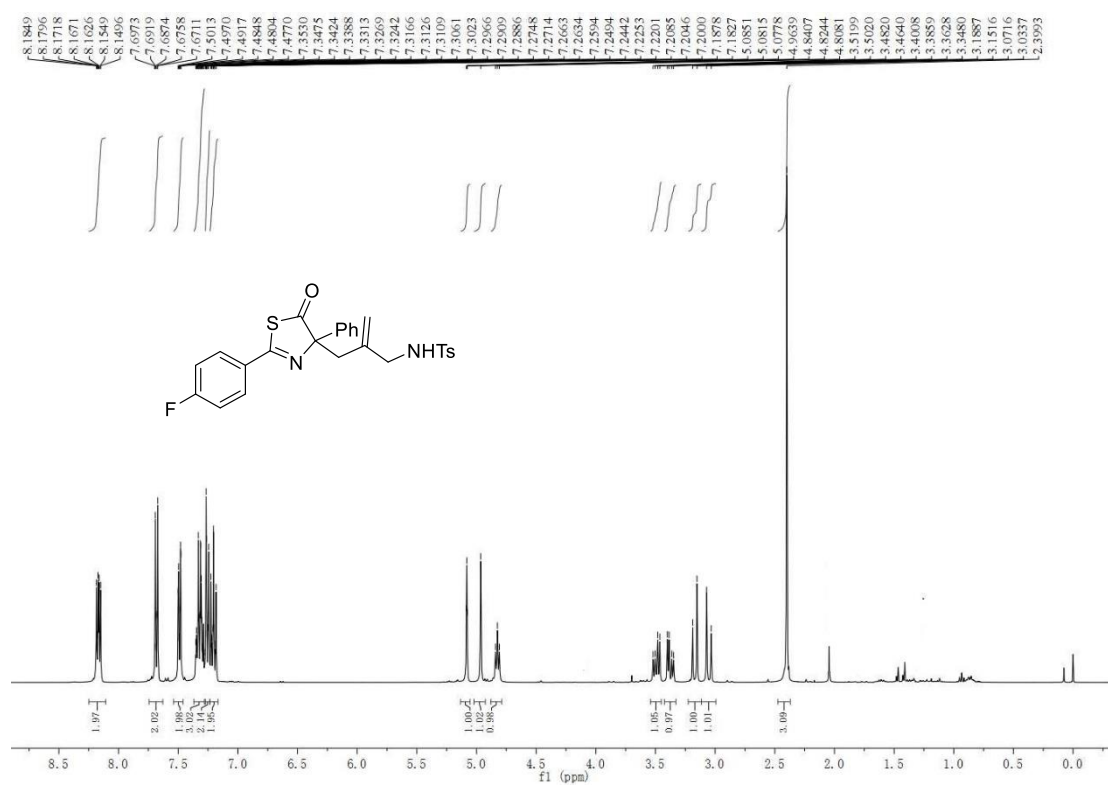
Identification code	5d
Empirical formula	C ₂₇ H ₂₅ ClN ₂ O ₄ S
Formula weight	509.00
Temperature/K	99.98(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.1642(2)
b/Å	11.1077(2)
c/Å	12.6071(2)
α/°	67.633(2)
β/°	85.5240(10)
γ/°	70.287(2)
Volume/Å ³	1237.06(4)
Z	2
ρ _{calc} /g/cm ³	1.366
μ/mm ⁻¹	2.460
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 ≤ h ≤ 10, -13 ≤ k ≤ 13, -15 ≤ l ≤ 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. ^1H and ^{13}C NMR spectra for compounds 3 and 5

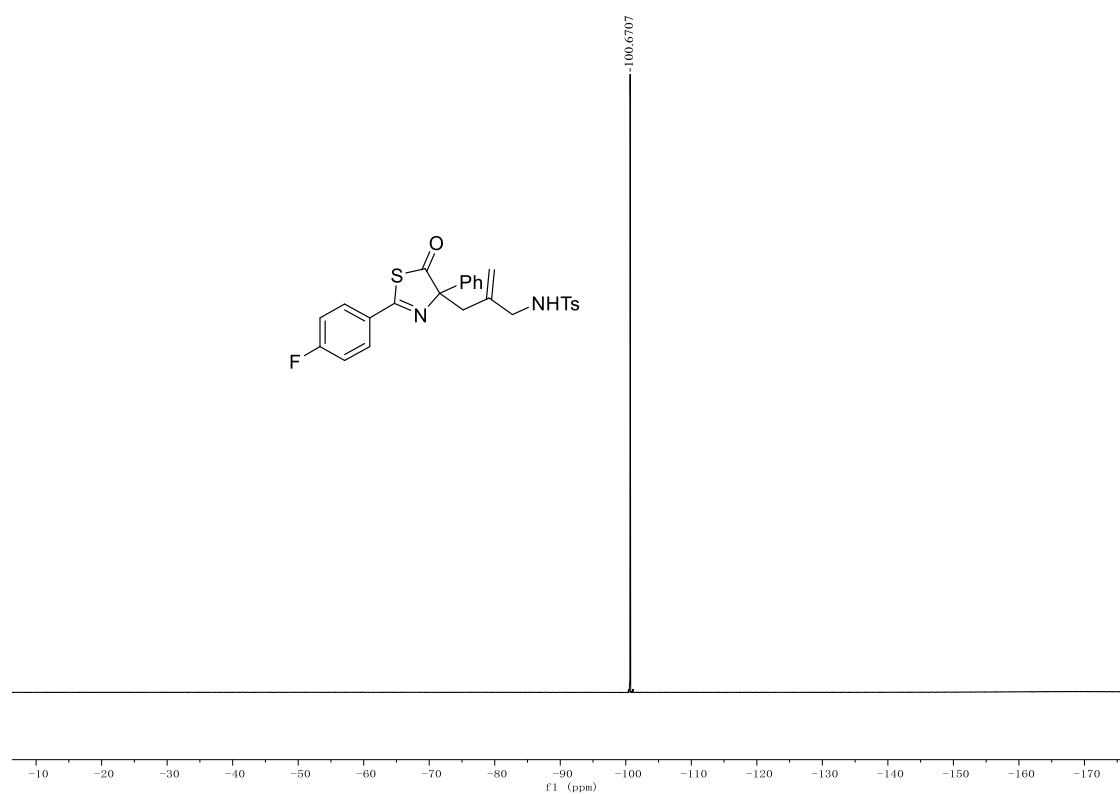
^1H and ^{13}C NMR spectra for compound 3a



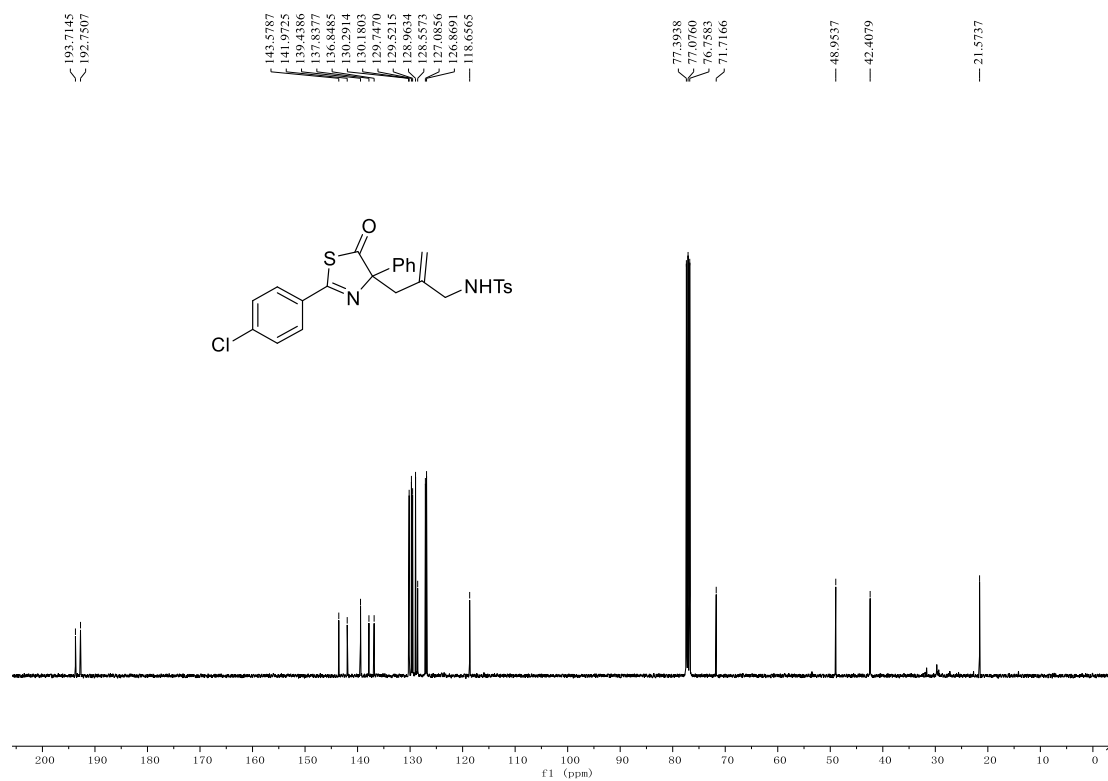
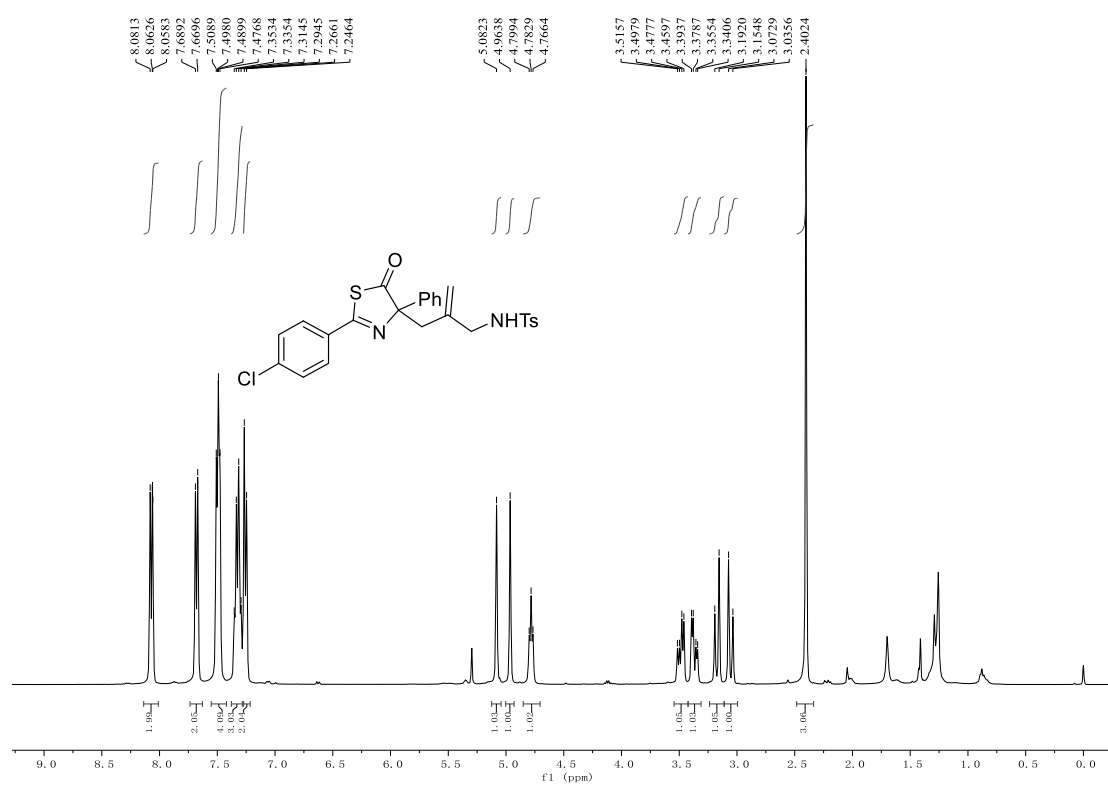
¹H and ¹³C NMR spectra for compound 3b



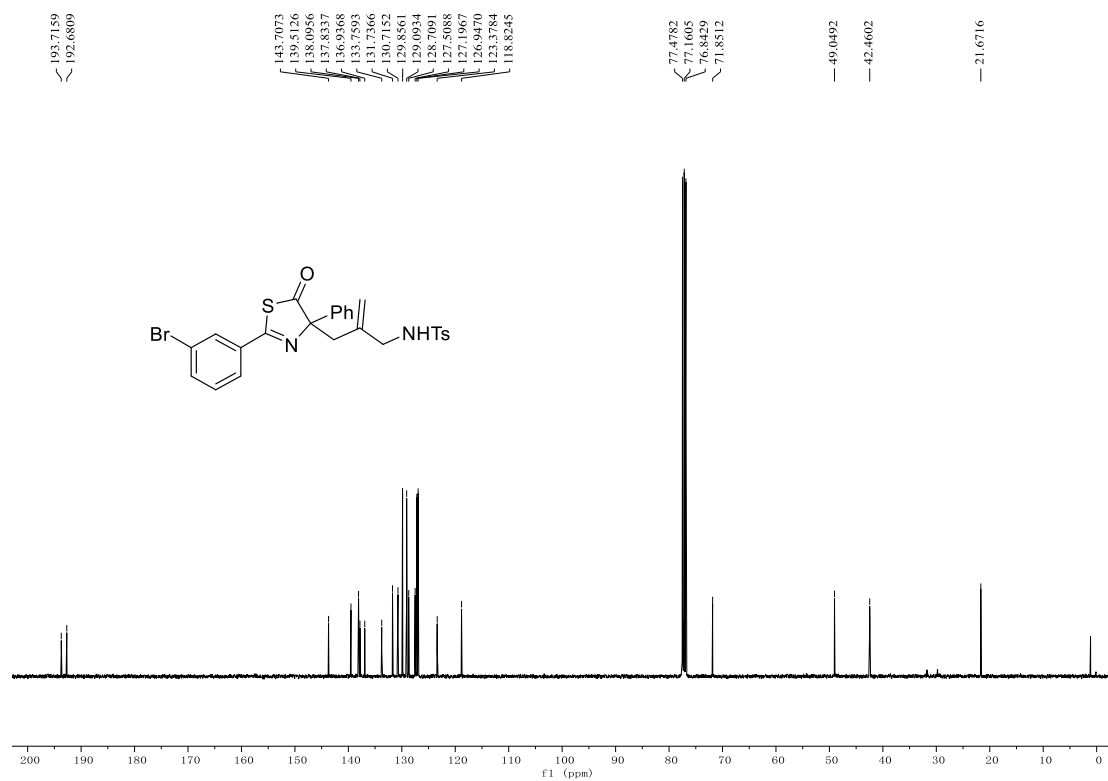
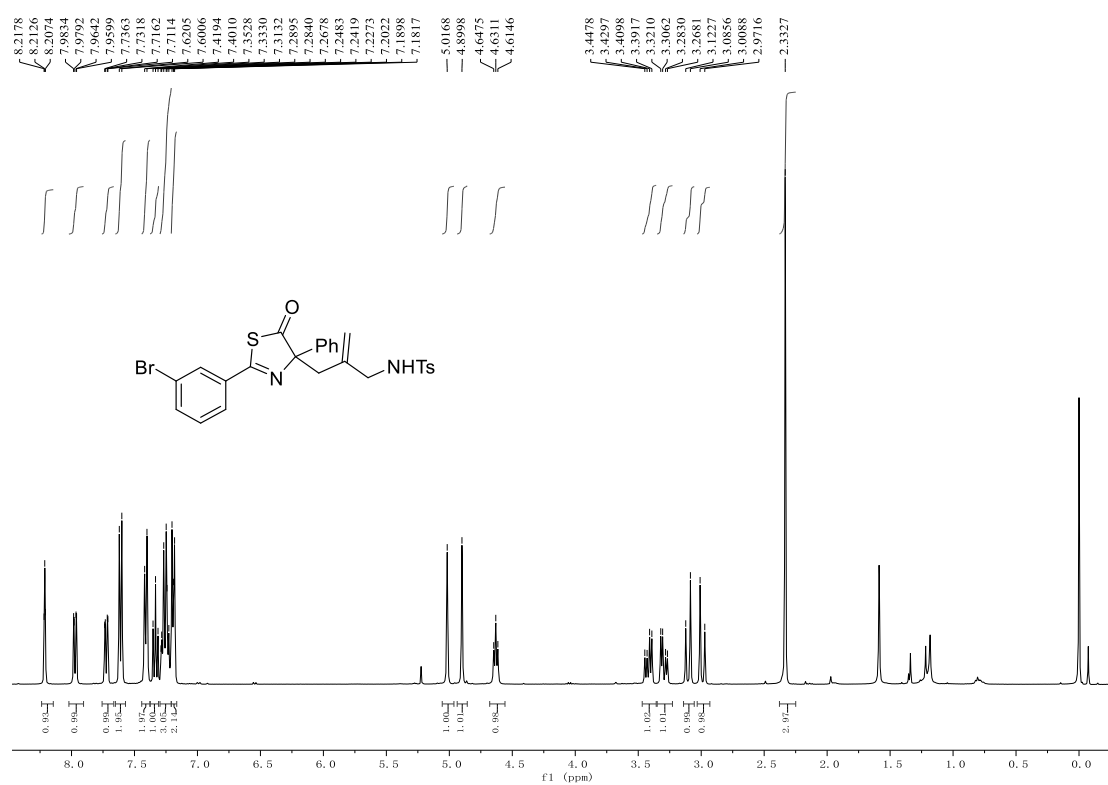
^{19}F NMR spectra for compound 3b



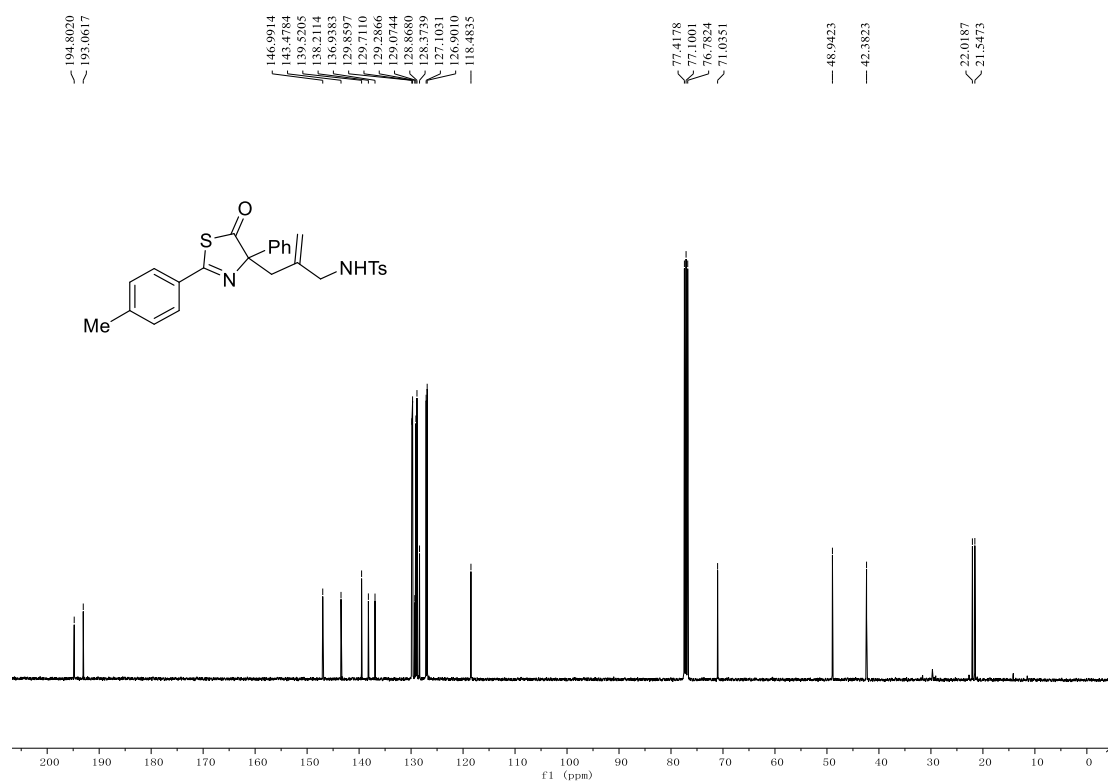
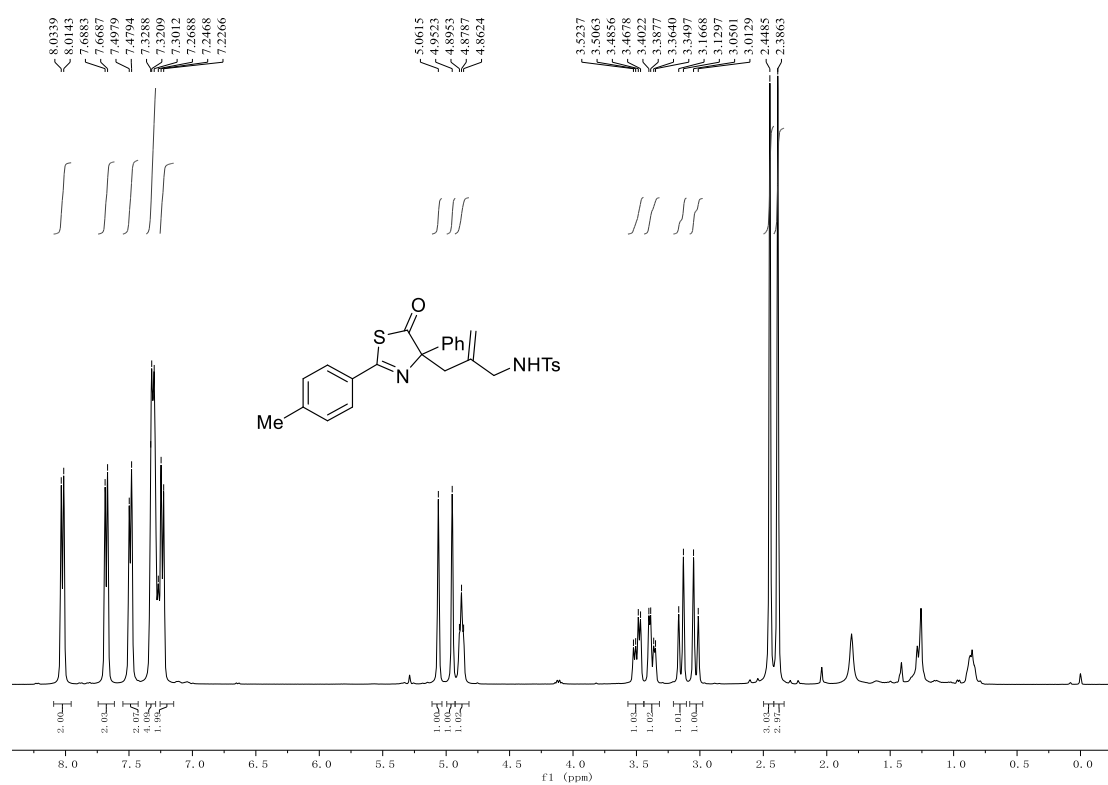
¹H and ¹³C NMR spectra for compound 3c



¹H and ¹³C NMR spectra for compound 3d



¹H and ¹³C NMR spectra for compound 3e



Chemical structure of compound 10: CC1(C)OC(=O)N1Cc2ccccc2

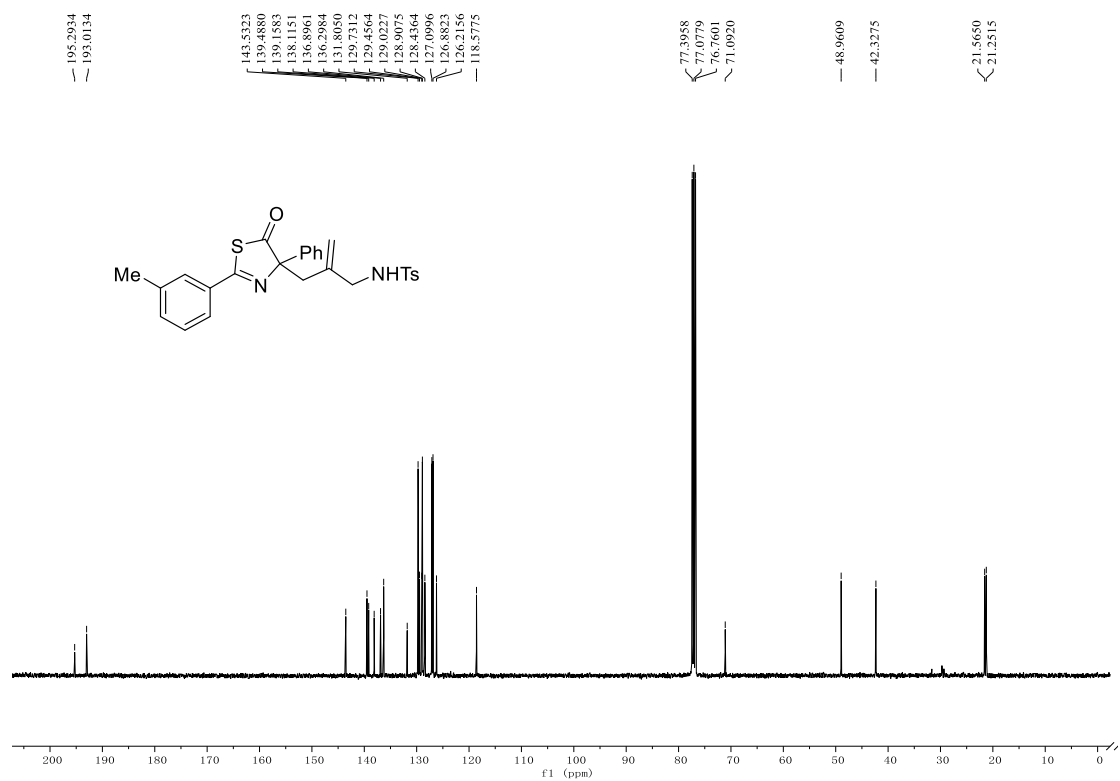
¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm, ranging from 0.0 to 8.5. The spectrum shows several peaks corresponding to the structure, with integration values provided for some of the signals.

Chemical shift data (ppm):

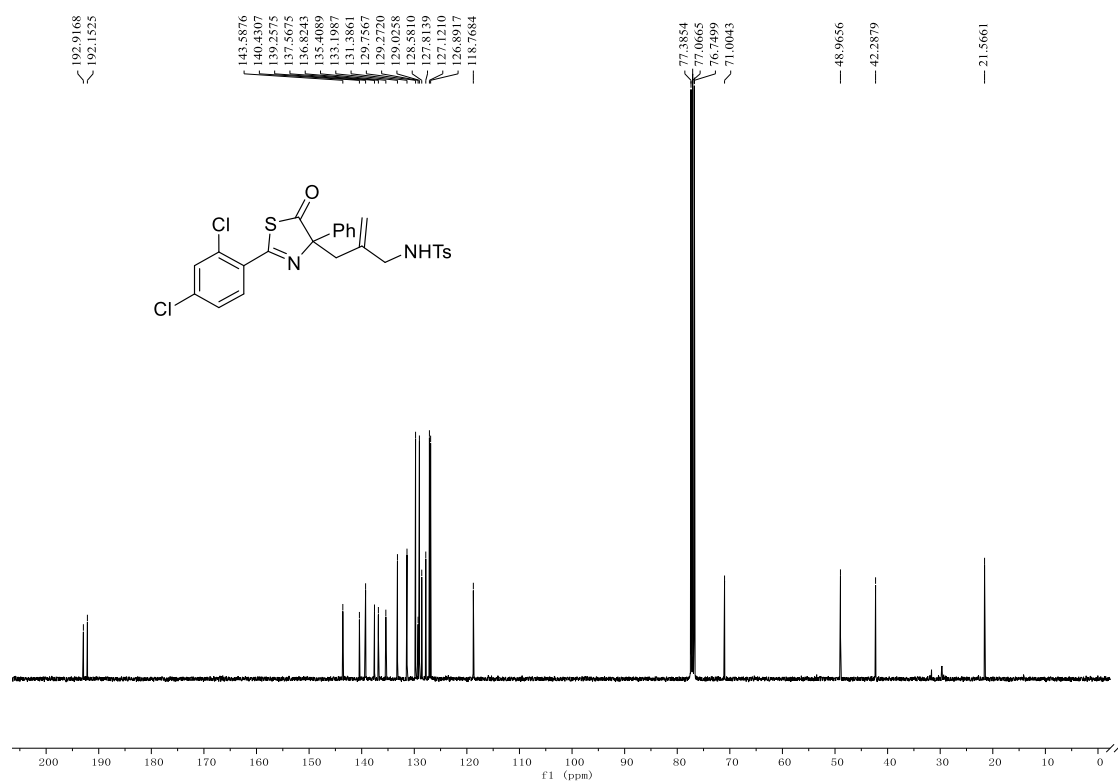
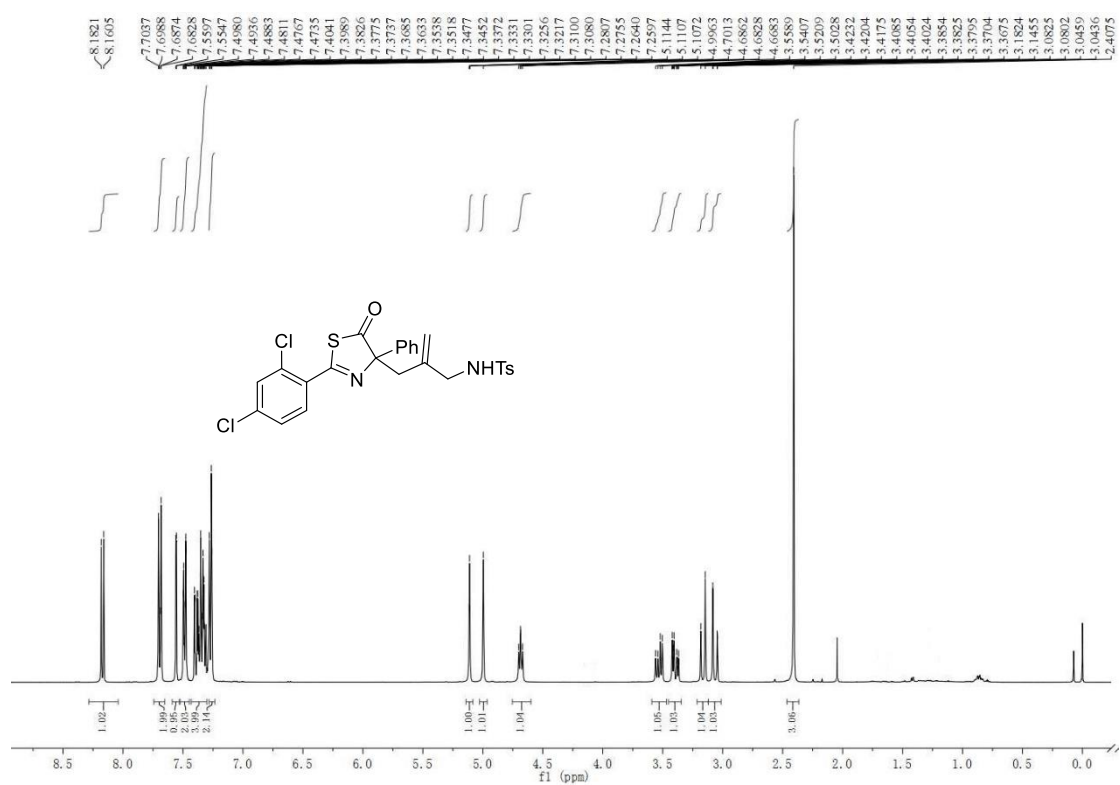
- 7.938, 7.9353, 7.9157, 7.9022, 7.8925, 7.9037, 7.8849, 7.4366, 7.4073, 7.3880, 7.3466, 7.3287, 7.3092, 7.3013, 7.2857, 7.2582, 7.2370
- 5.0741, 4.9720, 4.7626, 4.7461, 4.7297
- 3.5343, 3.5165, 3.4984, 3.4783, 3.4622, 3.3924, 3.3691, 3.3543, 3.1725, 3.1354, 3.0692, 3.0321, 2.4343, 2.3942

Integration values (from left to right):

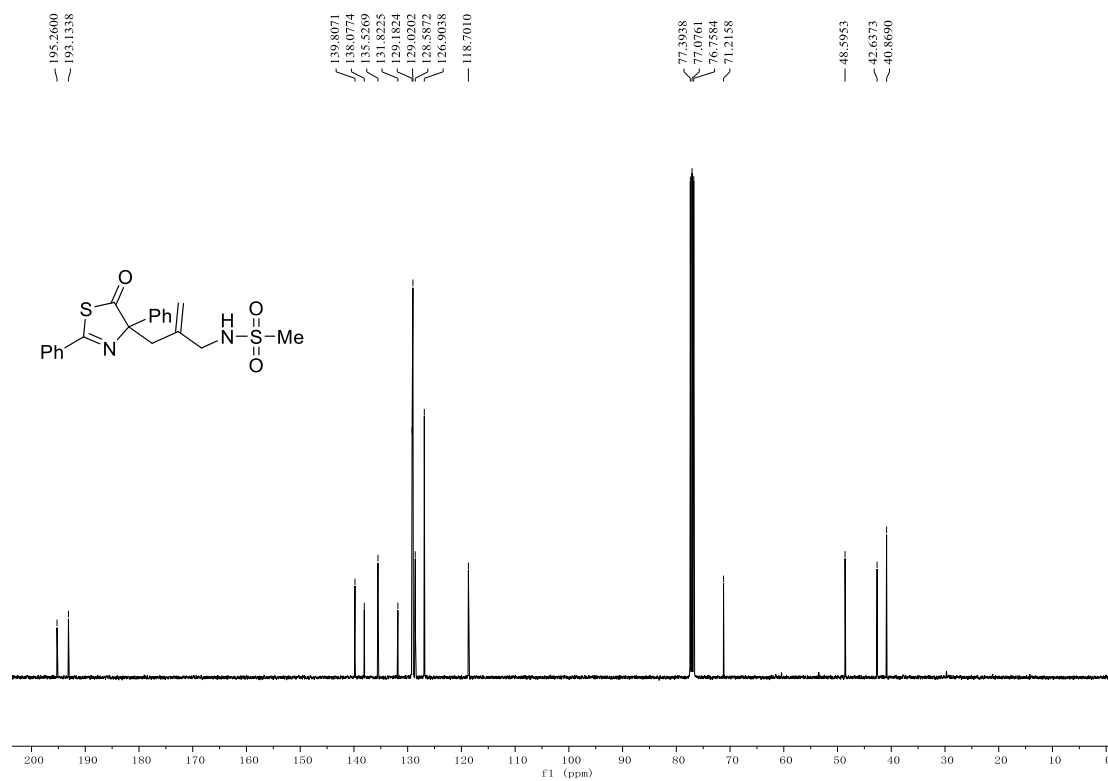
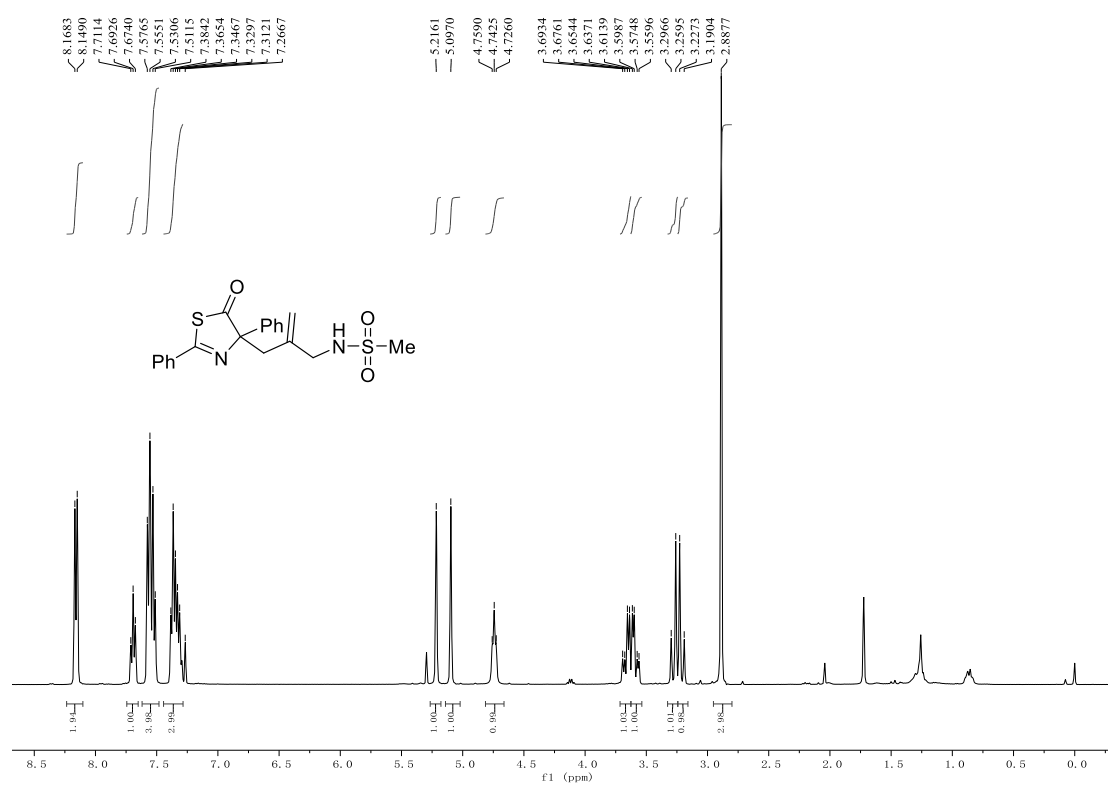
- 0.97, 1.00, 1.96, 2.98, 1.08, 2.27, 2.27
- 1.00, 0.98, 1.00
- 1.00, 1.00, 1.00, 0.99
- 3.06, 2.96



¹H and ¹³C NMR spectra for compound 3g



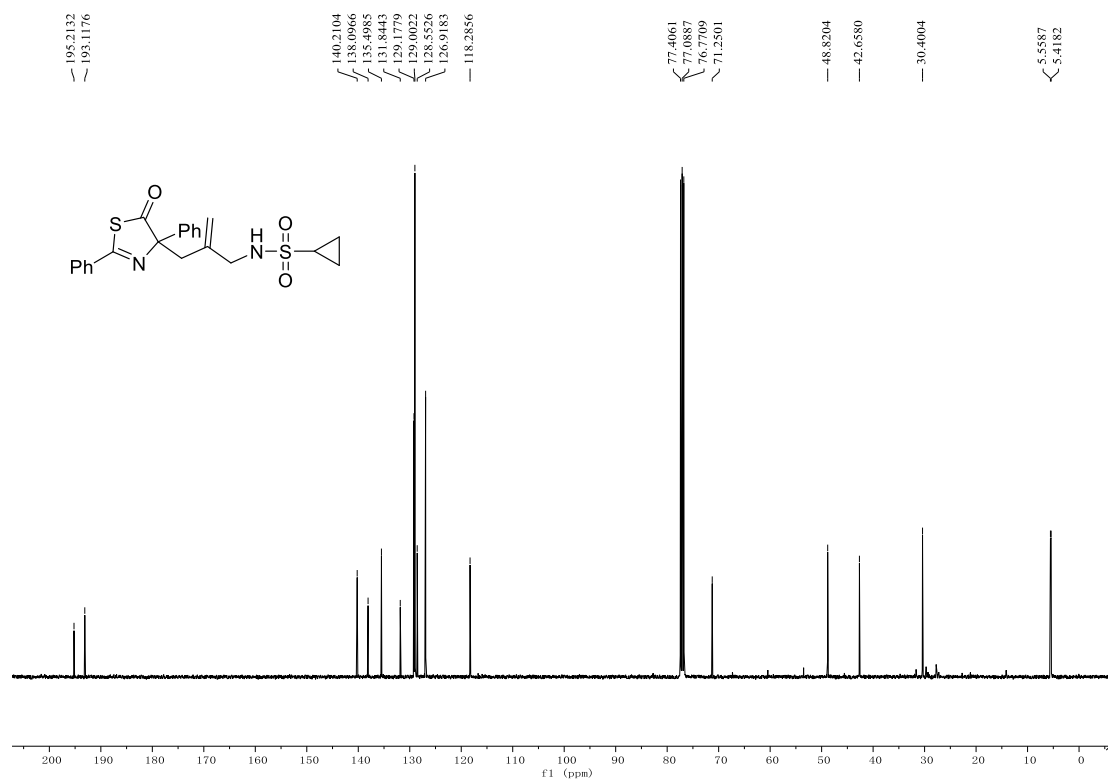
¹H and ¹³C NMR spectra for compound 3h



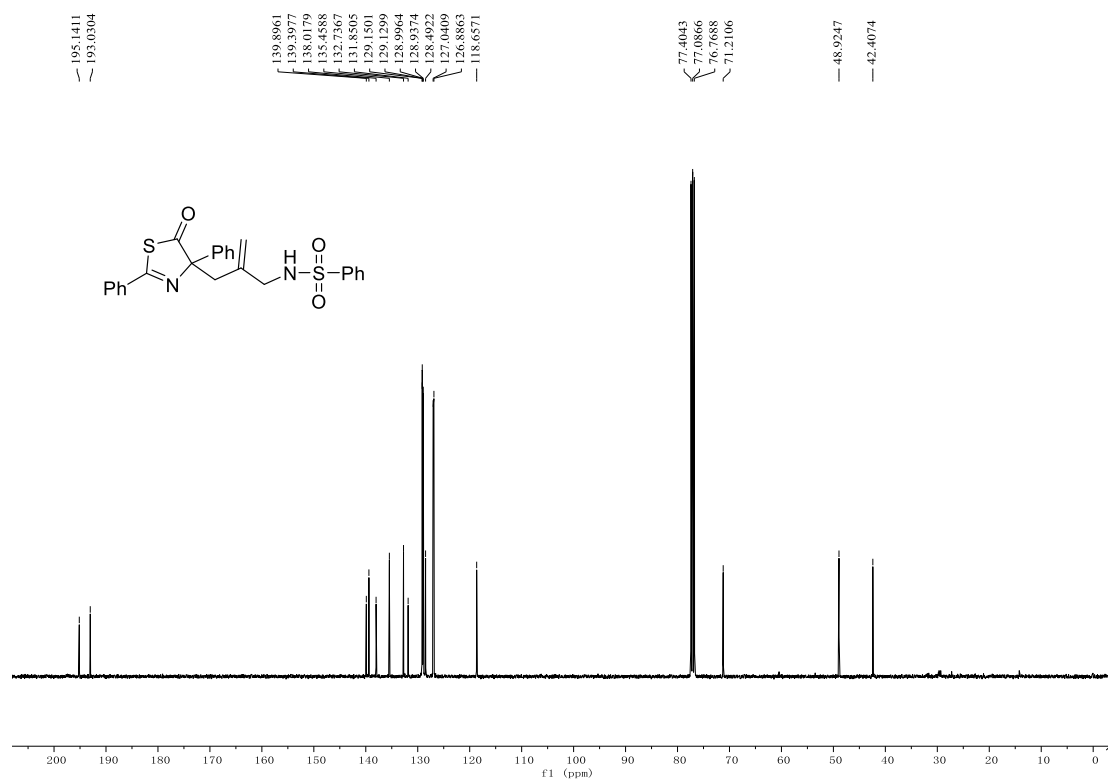
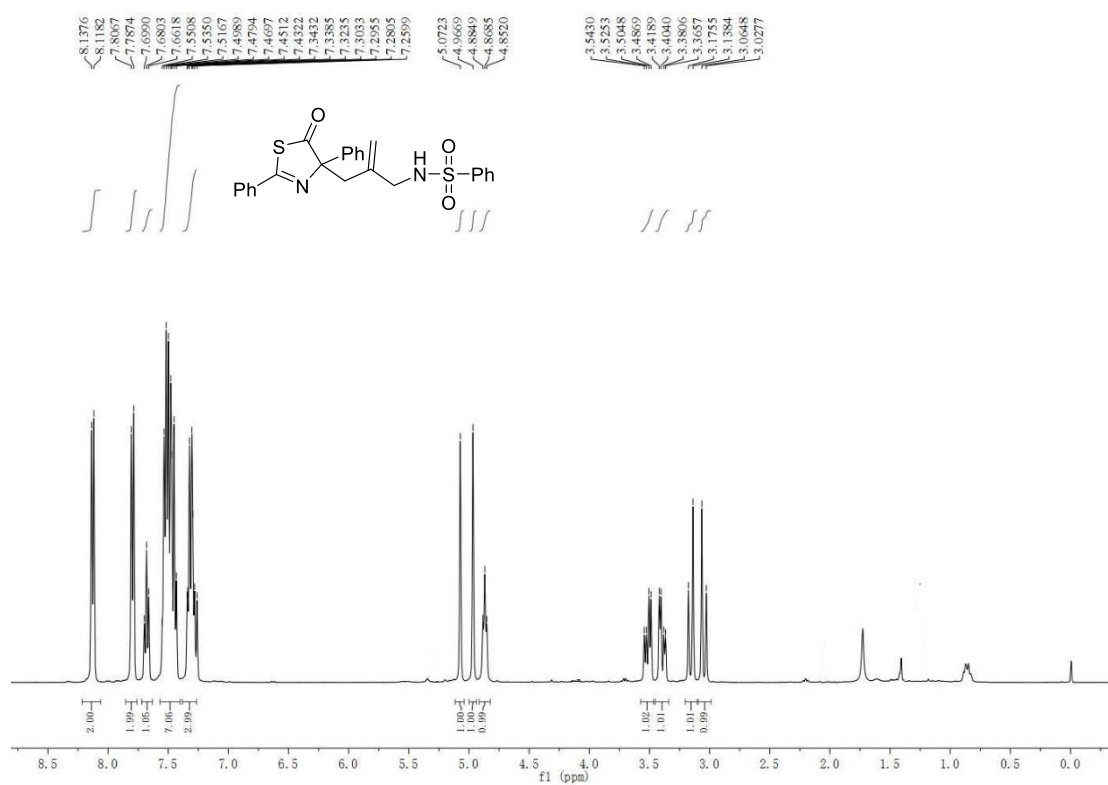
Chemical structure of compound 10 is shown above the spectrum. The spectrum displays peaks corresponding to the structure, with integration values indicated below the baseline. The x-axis represents the chemical shift in ppm, ranging from 0.0 to 8.5.

Peak list (ppm): 8.1738, 8.1545, 7.7126, 7.6938, 7.6751, 7.5832, 7.5636, 7.5520, 7.5332, 7.5141, 7.3877, 7.3689, 7.3470, 7.3280, 7.3115, 7.2928, 7.2680, 5.2241, 5.0807, 4.6493, 4.6331, 4.6171, 3.7141, 3.6968, 3.6748, 3.6574, 3.6356, 3.6204, 3.5964, 3.5813, 3.3212, 3.2841, 3.2228, 3.1957, 2.3686, 2.3607, 2.3491, 2.3369, 2.3289, 1.1209, 1.1079, 1.0901, 1.0804, 0.9305, 0.9104.

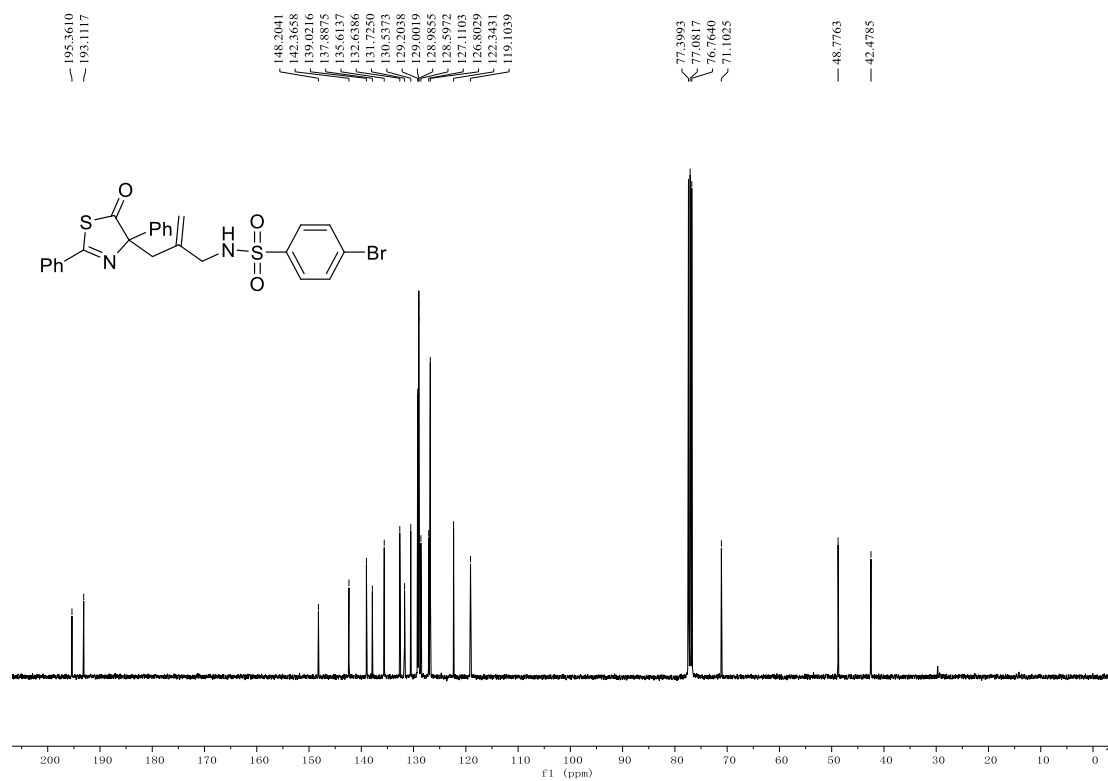
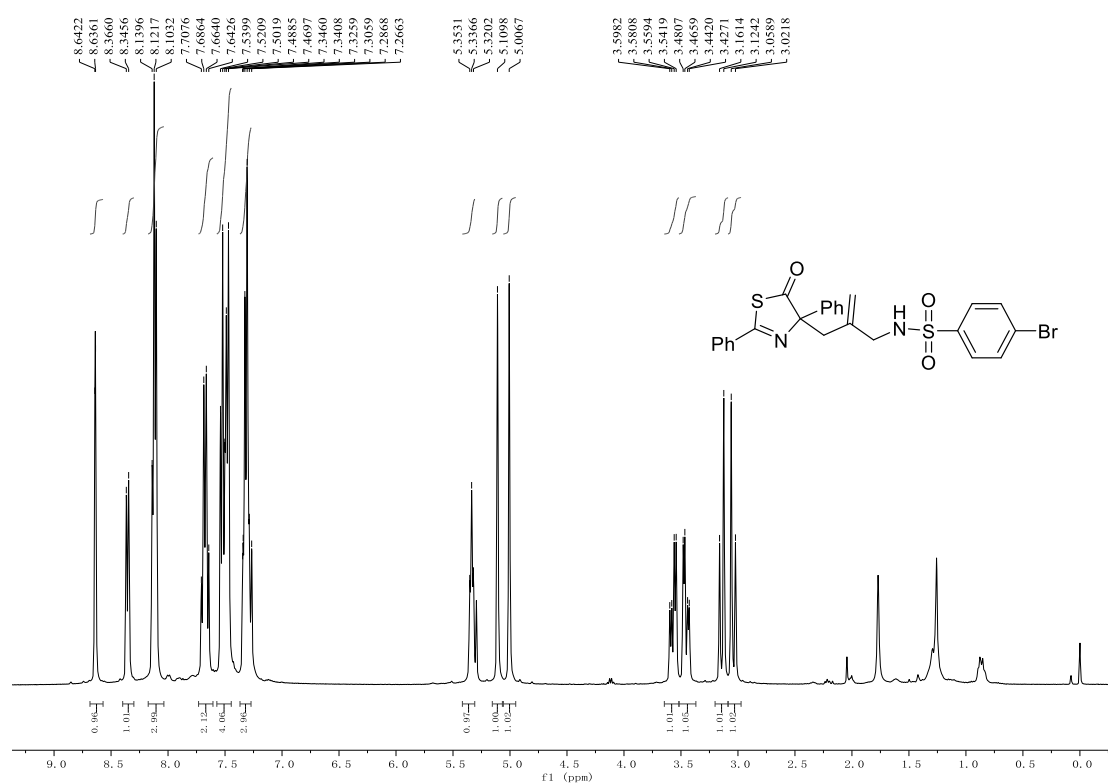
Integration values (from left to right): 2.00, 1.02, 4.06, 3.05, 1.04, 1.00, 1.07, 2.06, 1.00, 1.07, 2.16, 2.21.



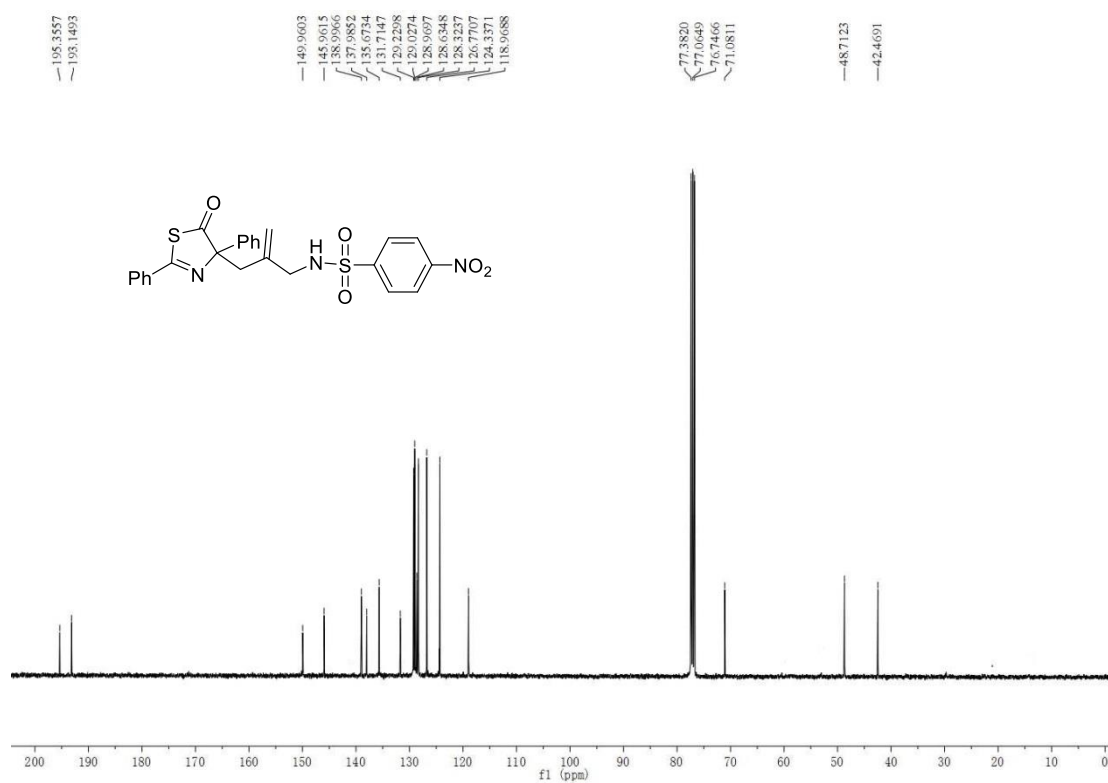
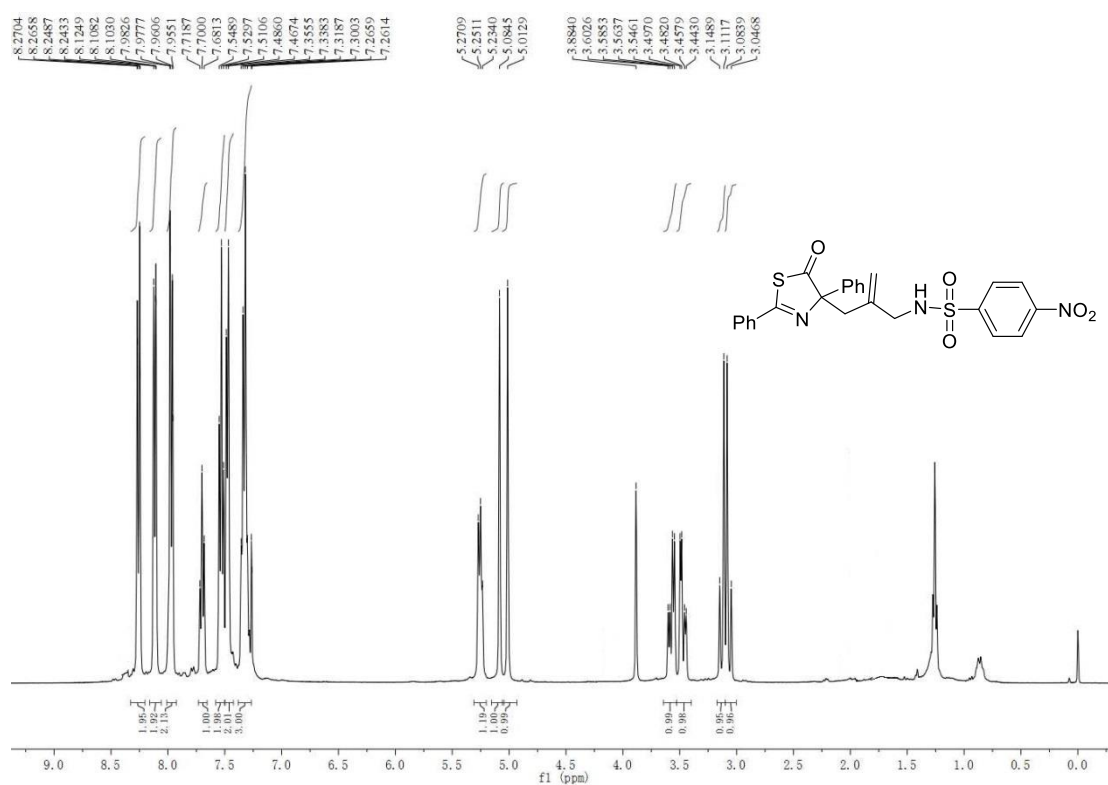
¹H and ¹³C NMR spectra for compound 3j



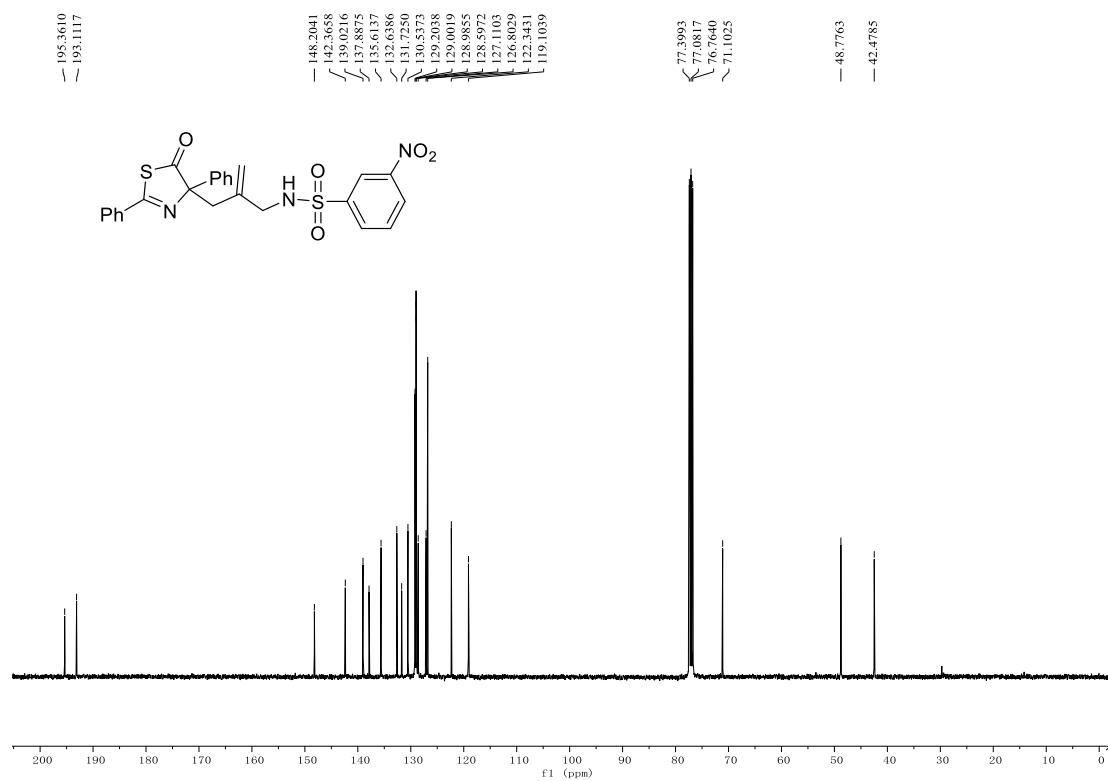
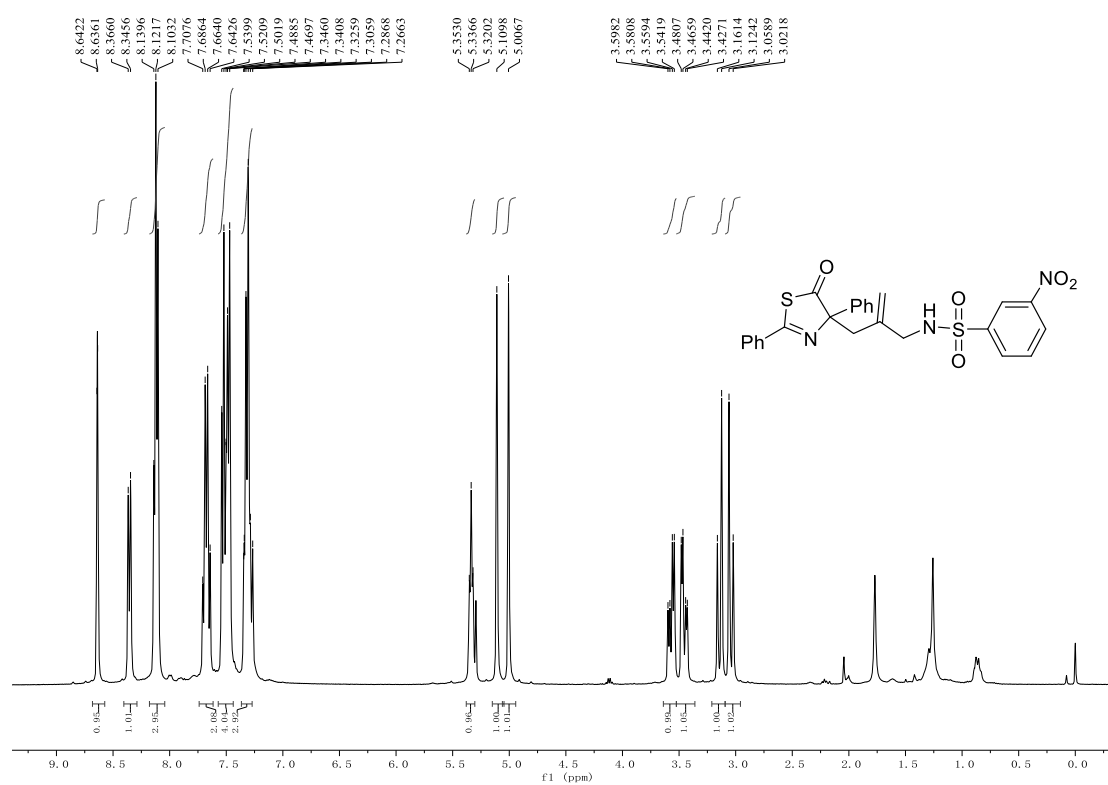
¹H and ¹³C NMR spectra for compound 3k



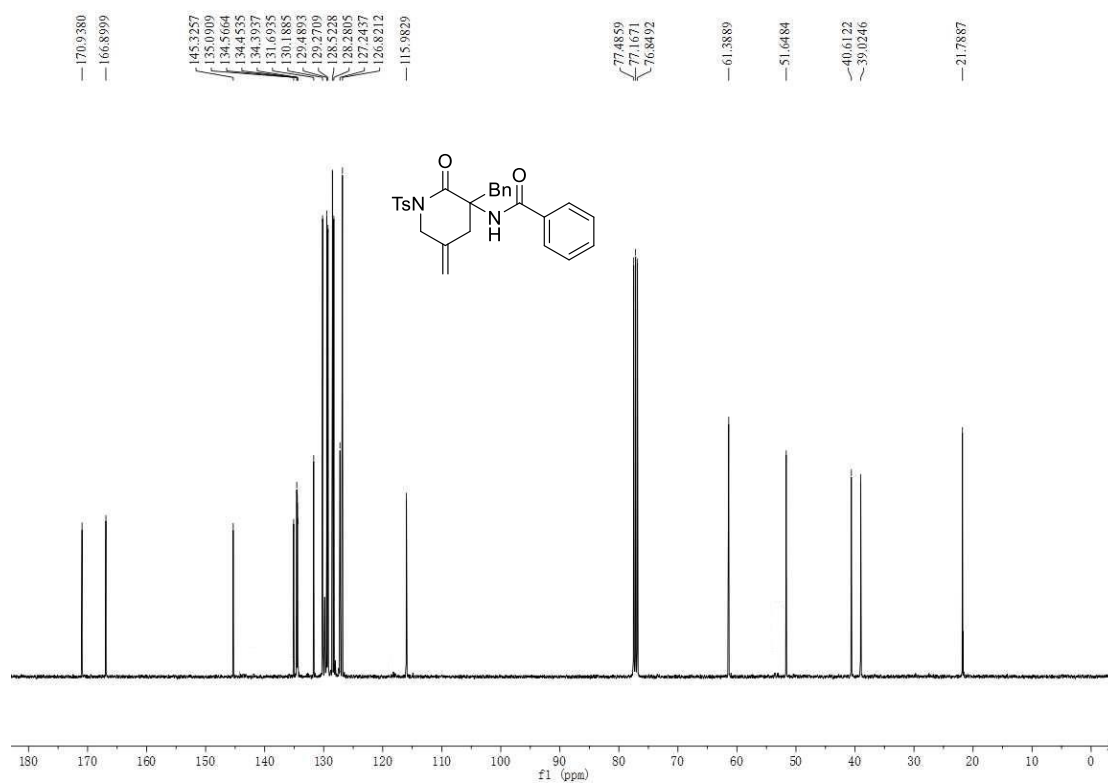
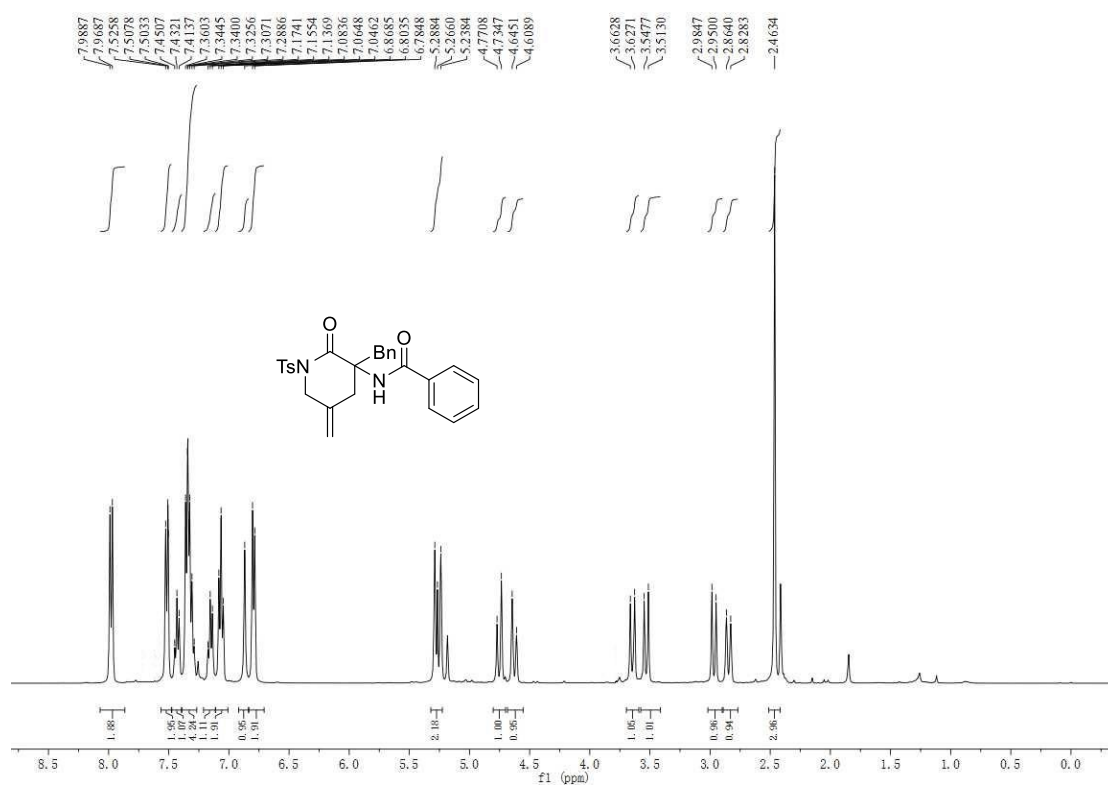
¹H and ¹³C NMR spectra for compound 3l



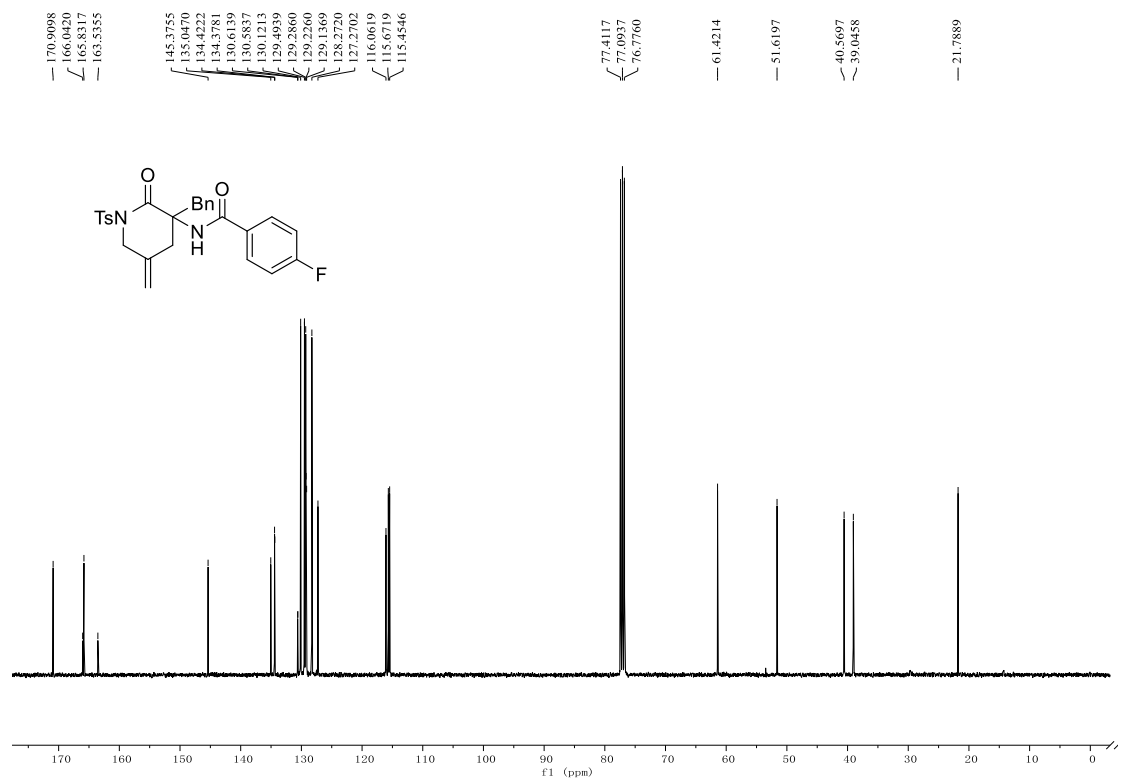
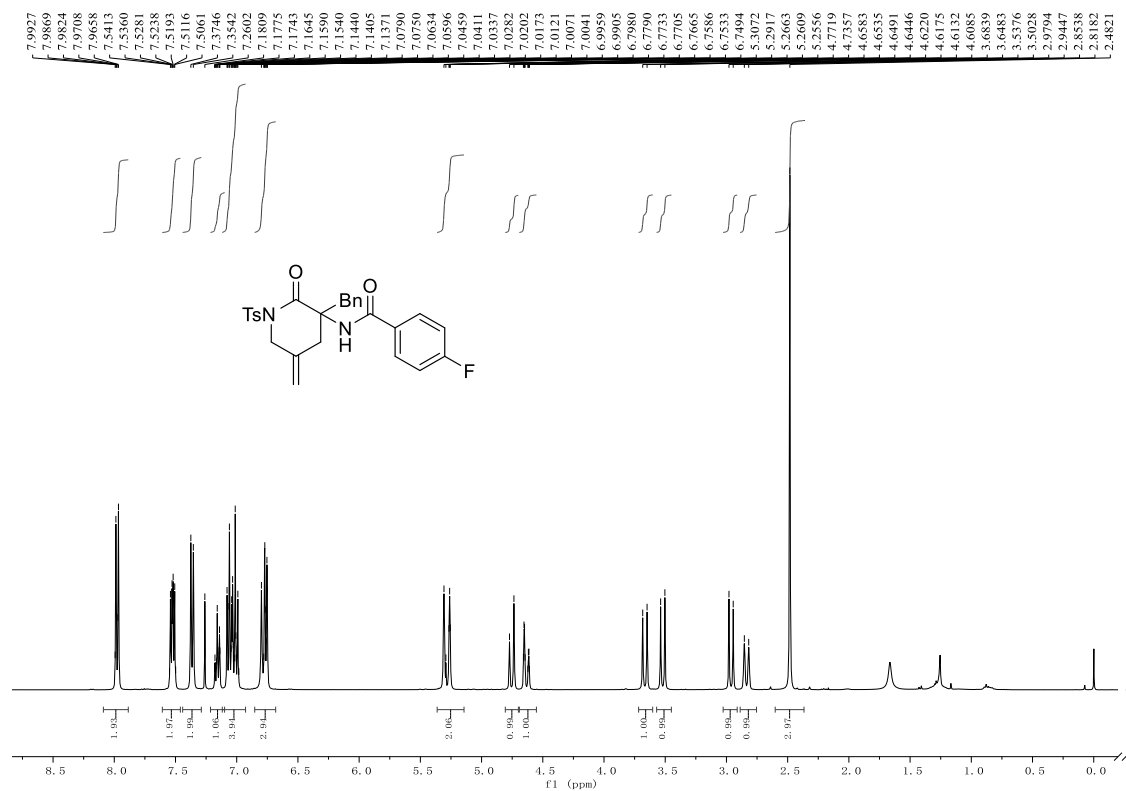
^1H and ^{13}C NMR spectra for compound 3m



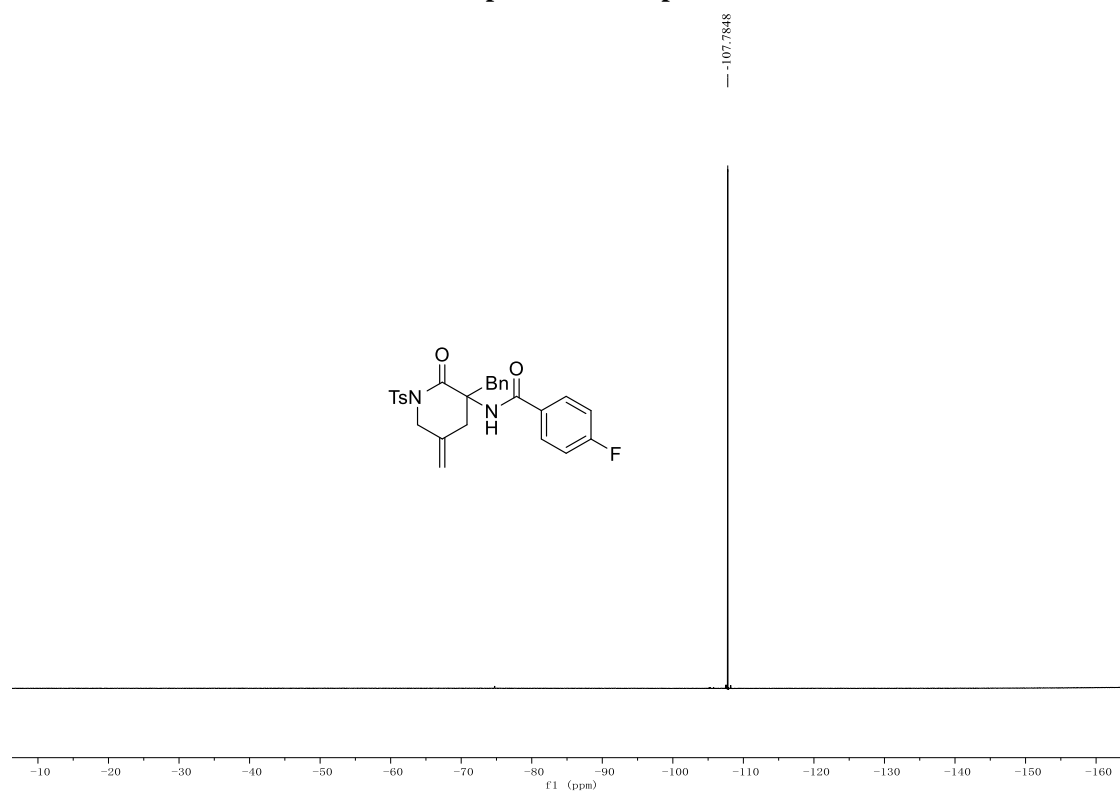
^1H and ^{13}C NMR spectra for compound 5a



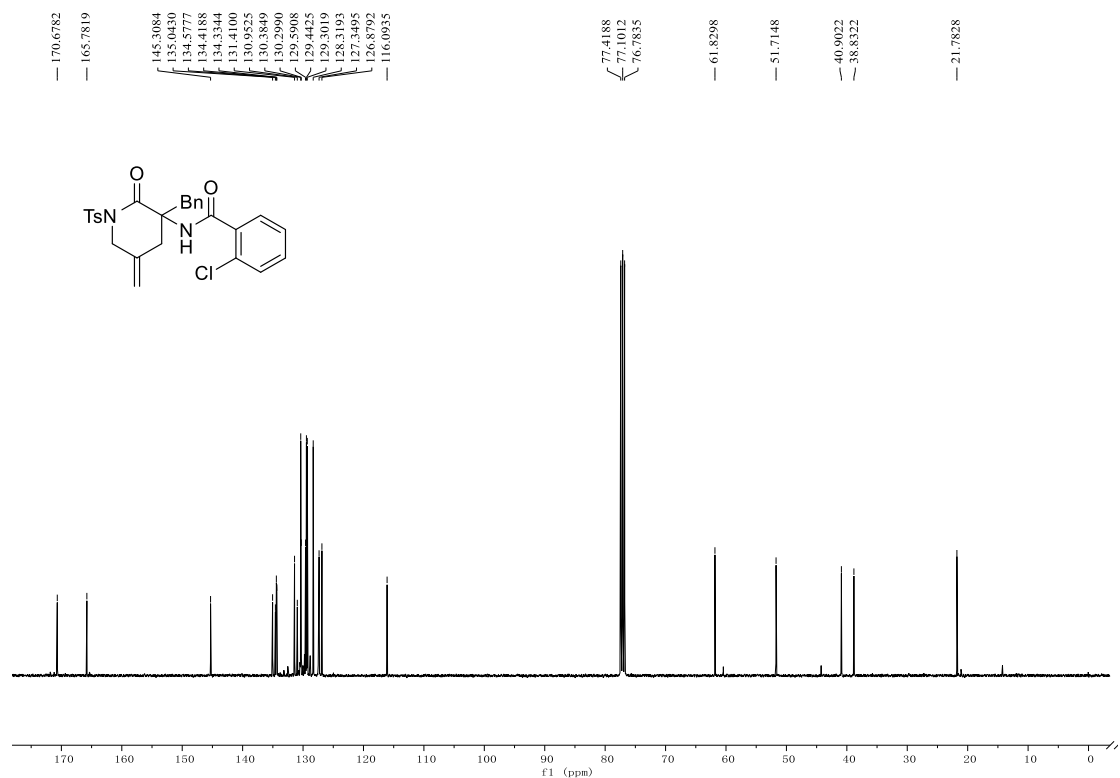
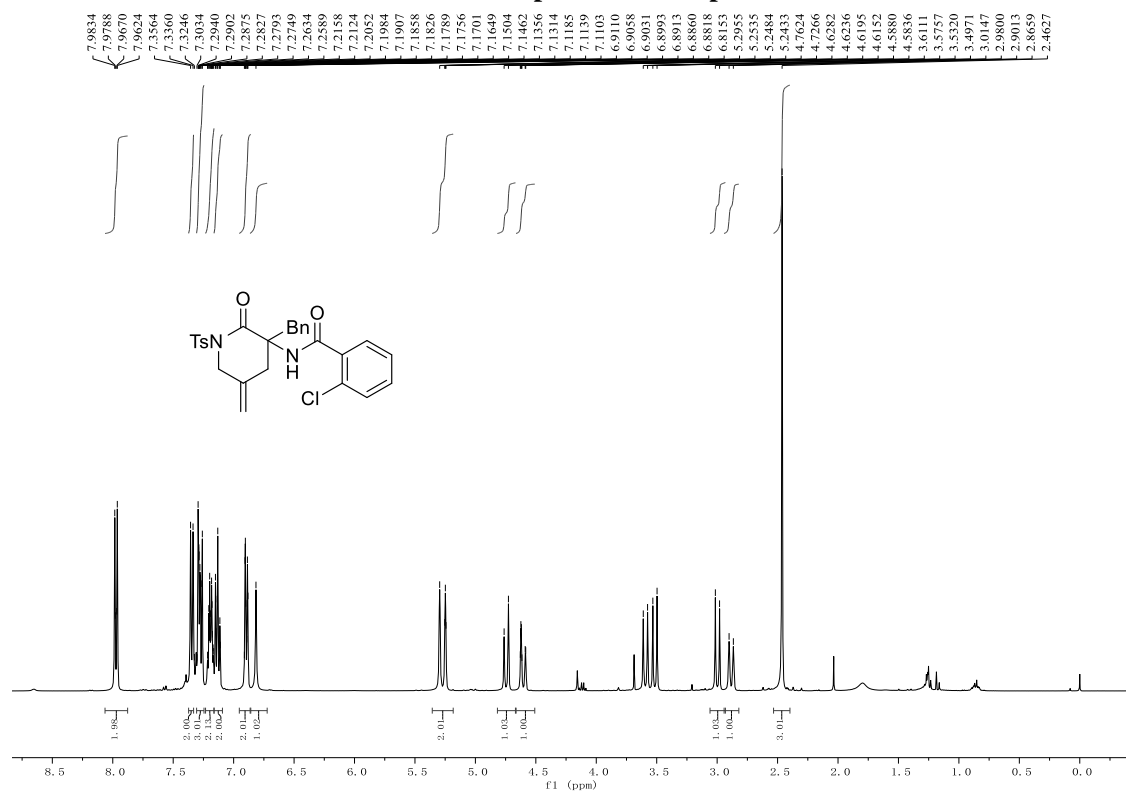
¹H and ¹³C NMR spectra for compound 5b



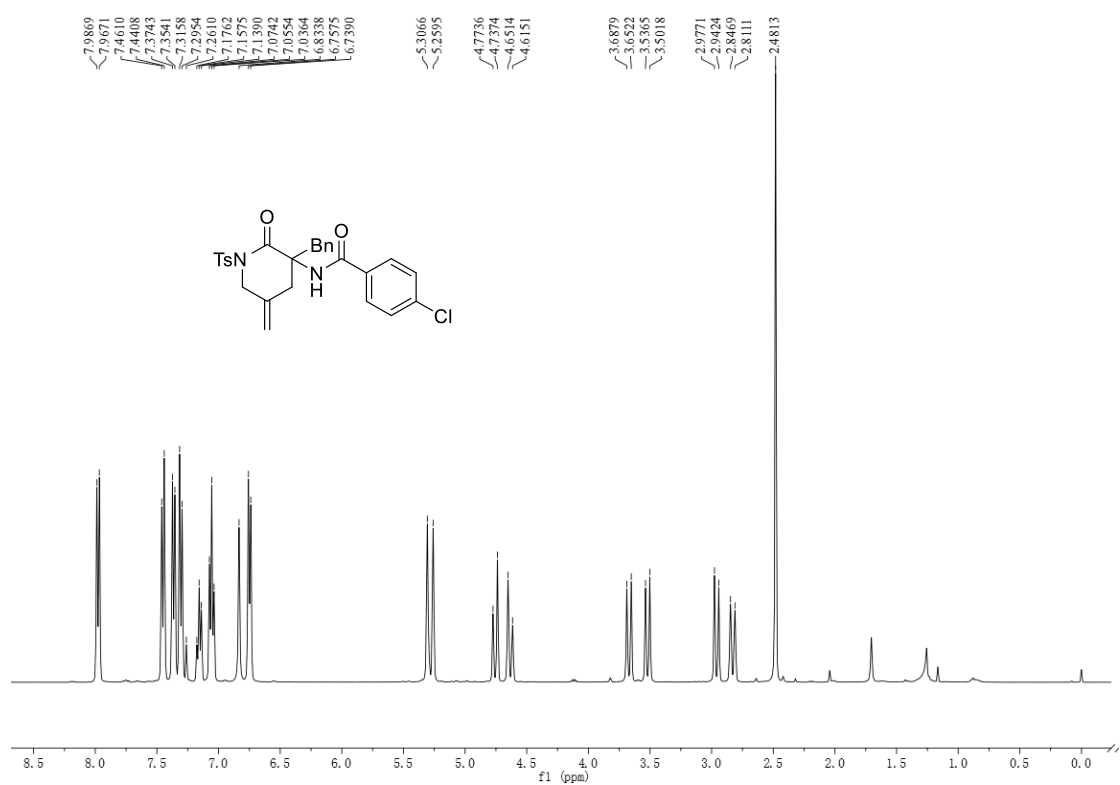
^{19}F NMR spectra for compound 5b



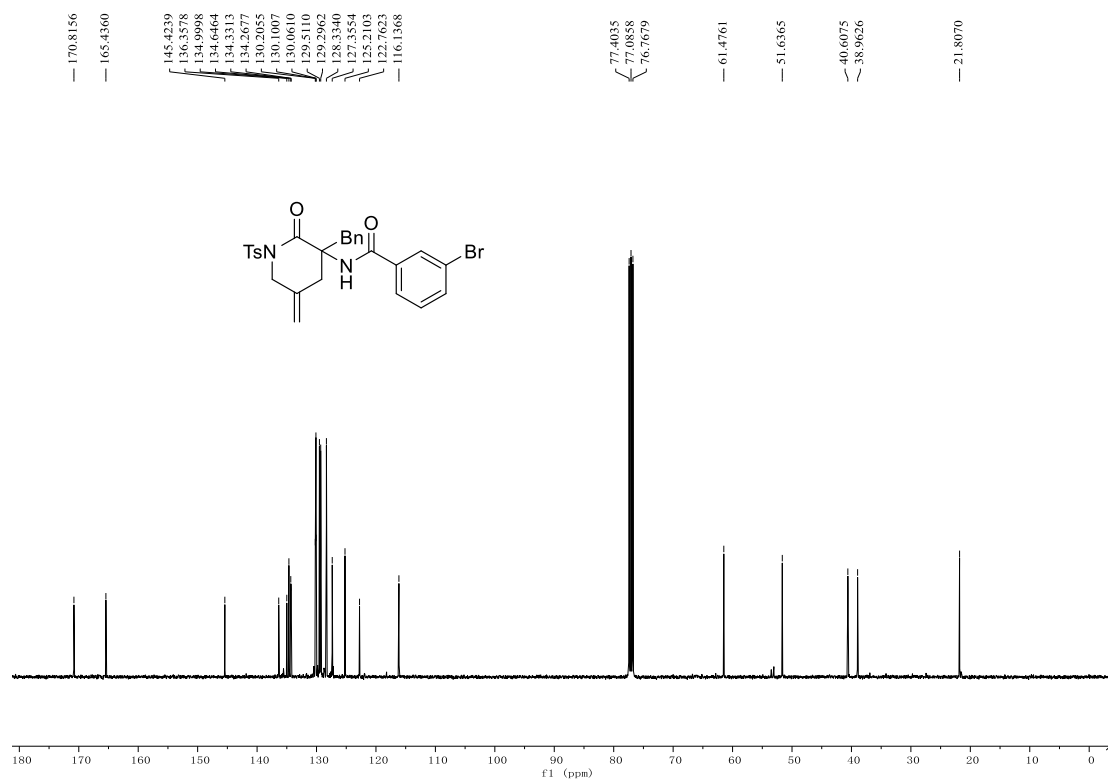
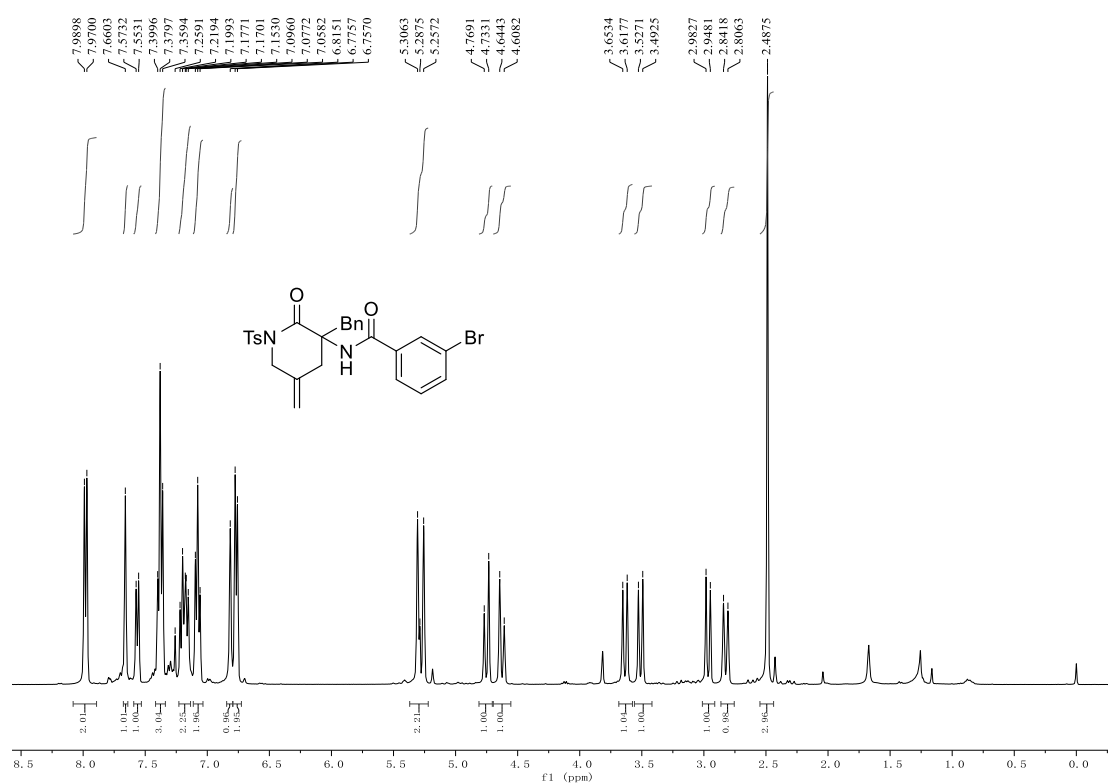
¹H and ¹³C NMR spectra for compound 5c



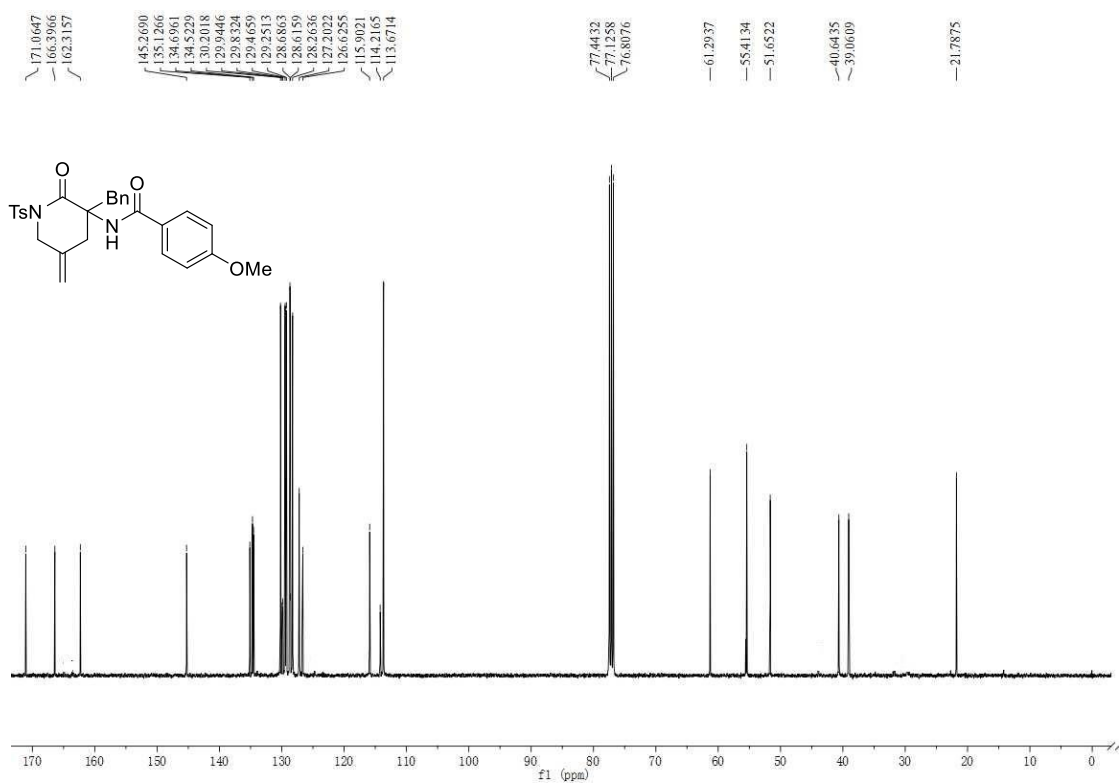
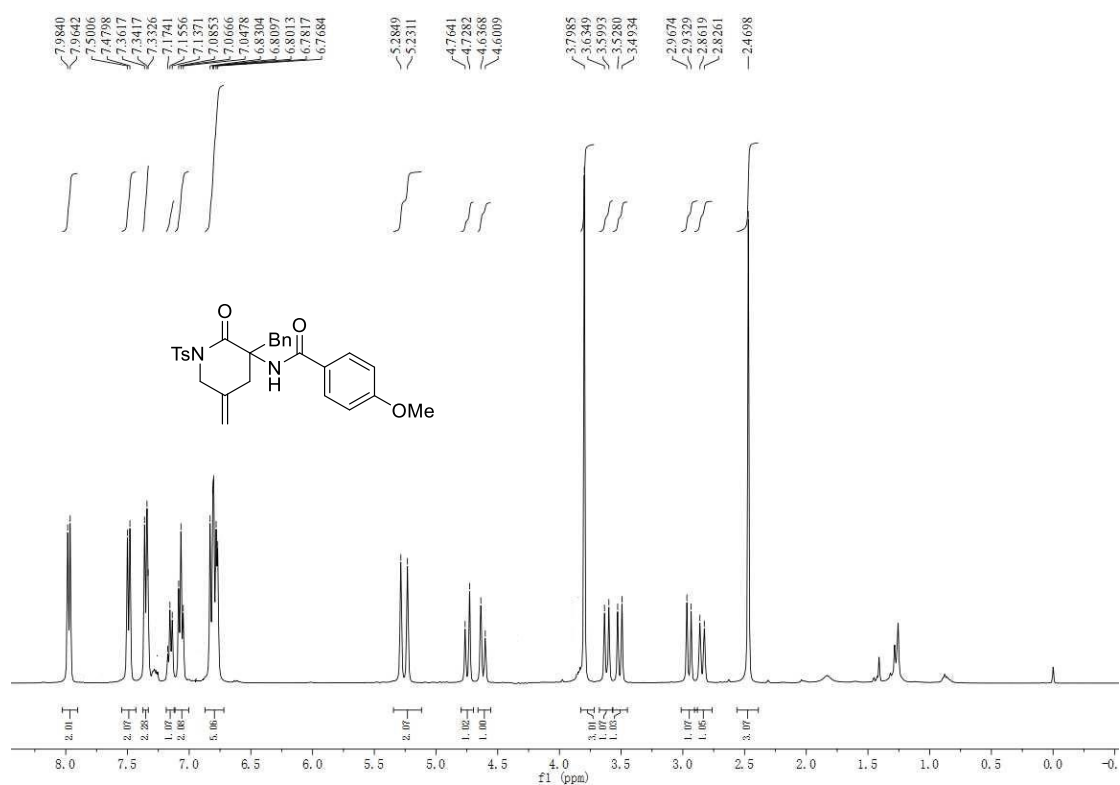
^1H and ^{13}C NMR spectra for compound 5d



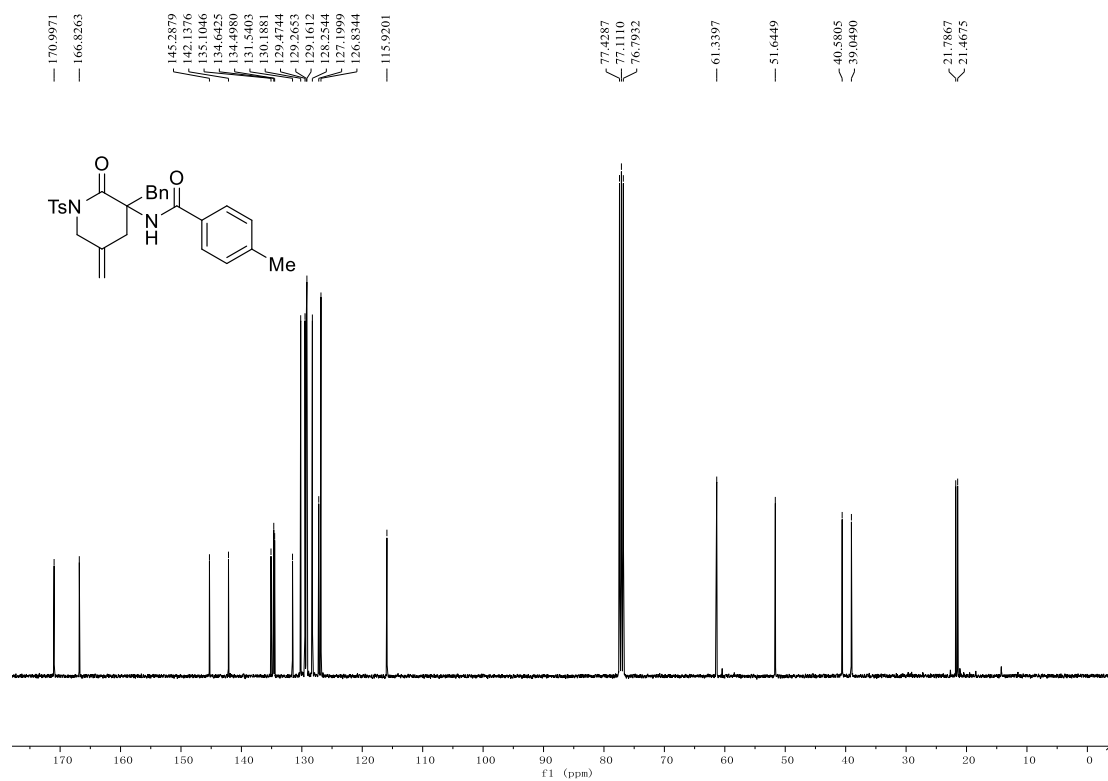
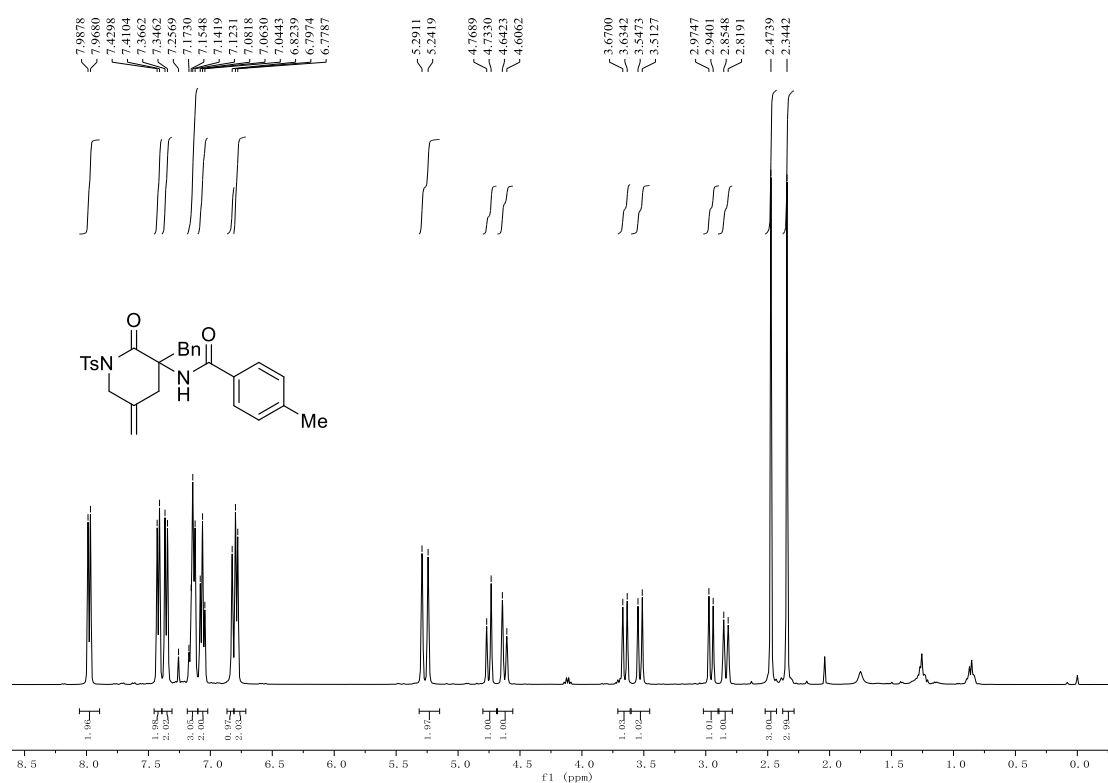
¹H and ¹³C NMR spectra for compound 5e



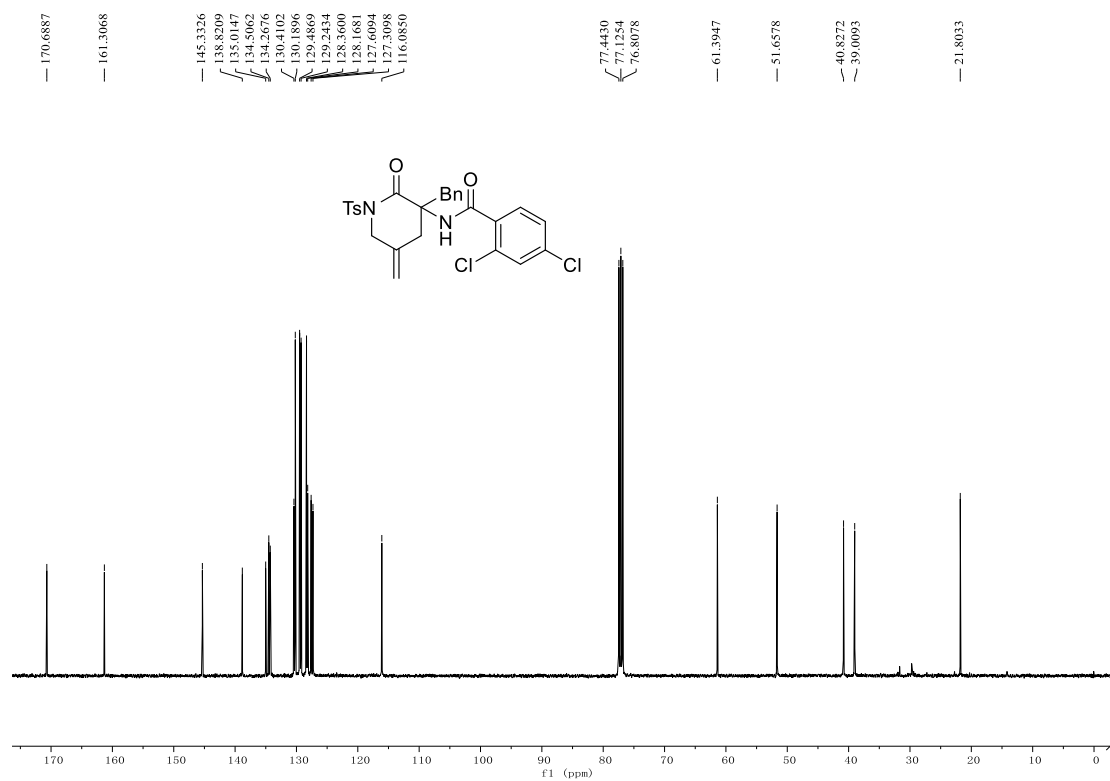
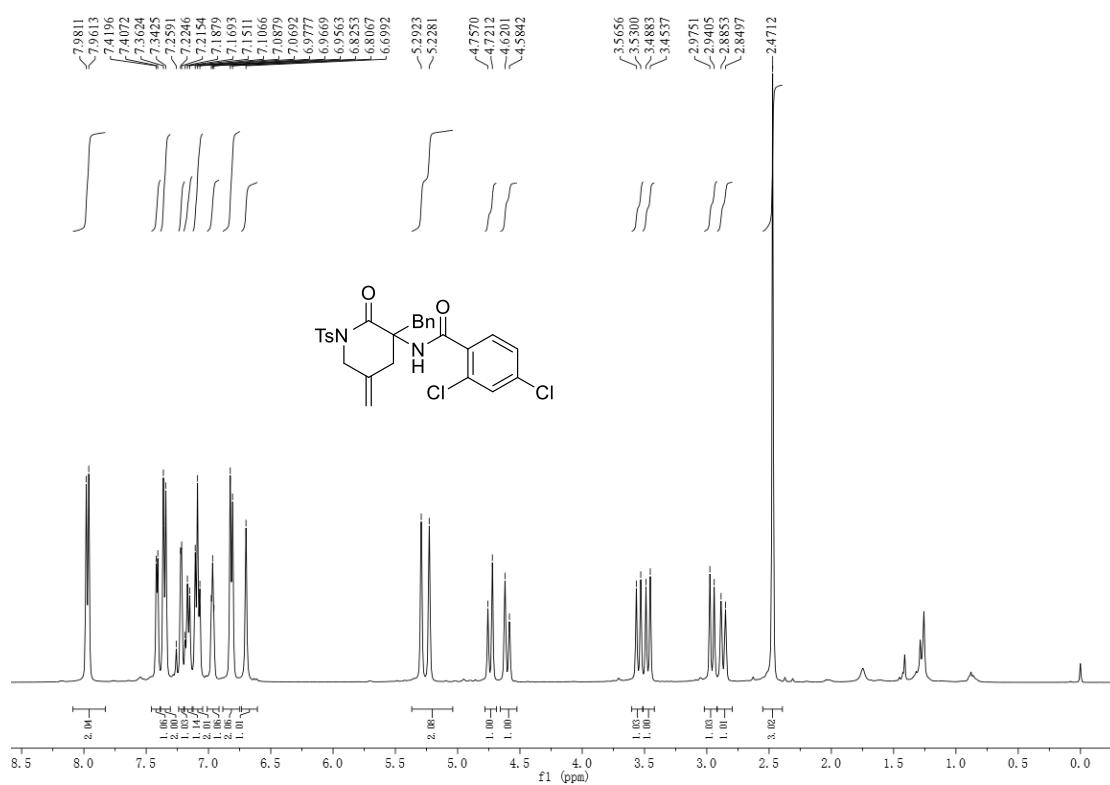
¹H and ¹³C NMR spectra for compound 5f



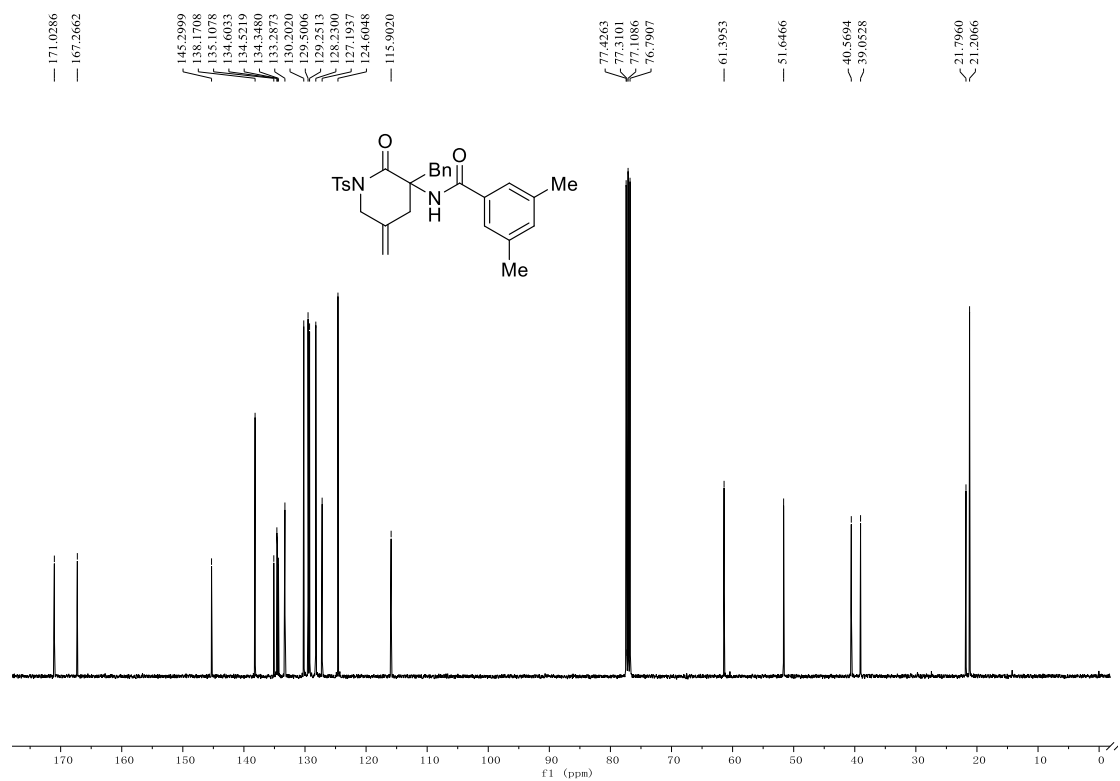
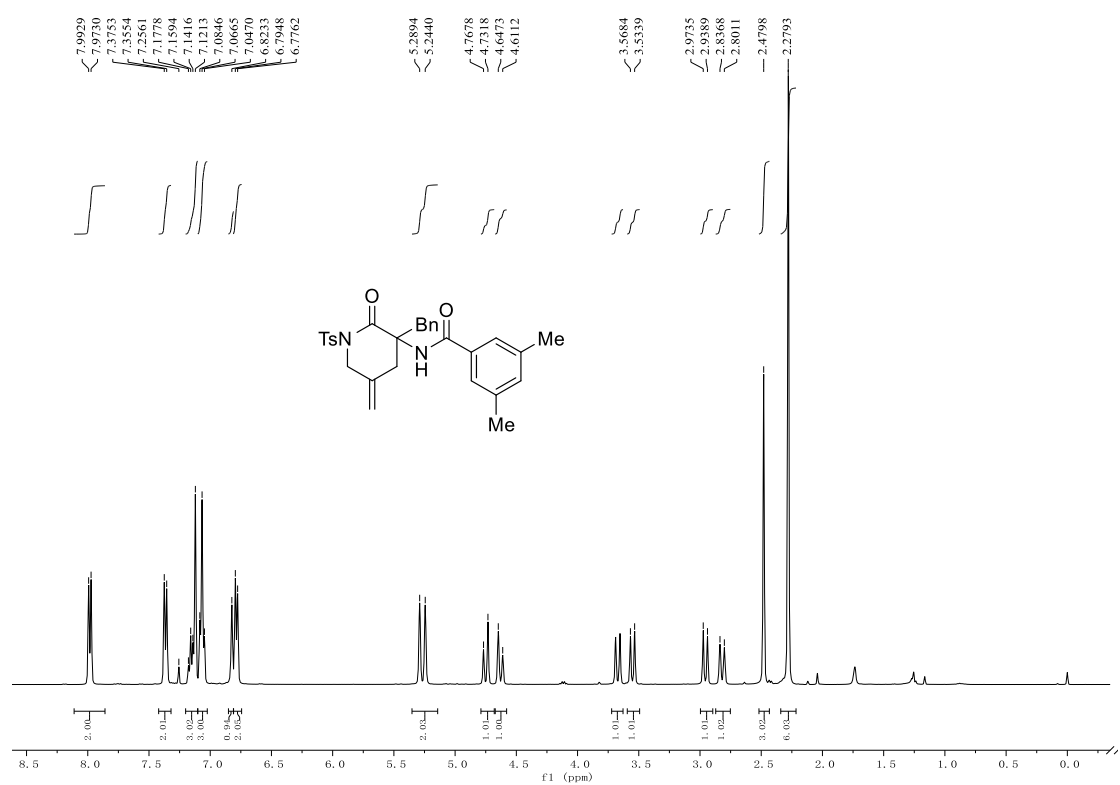
¹H and ¹³C NMR spectra for compound 5g



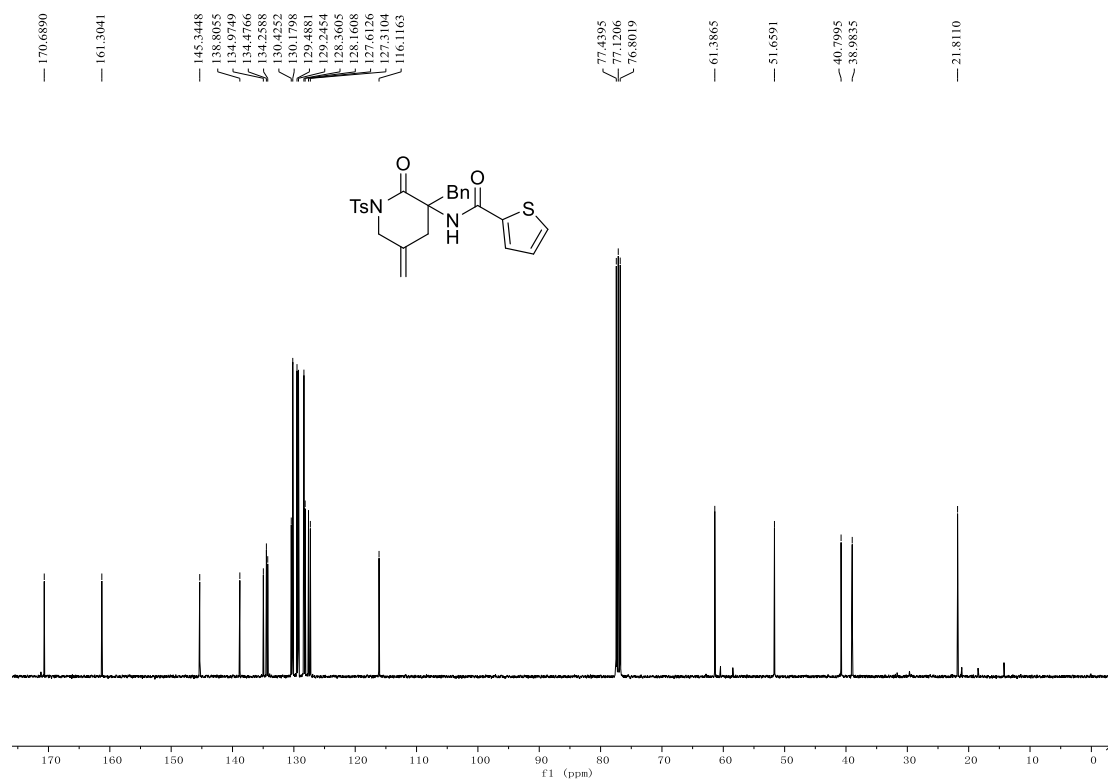
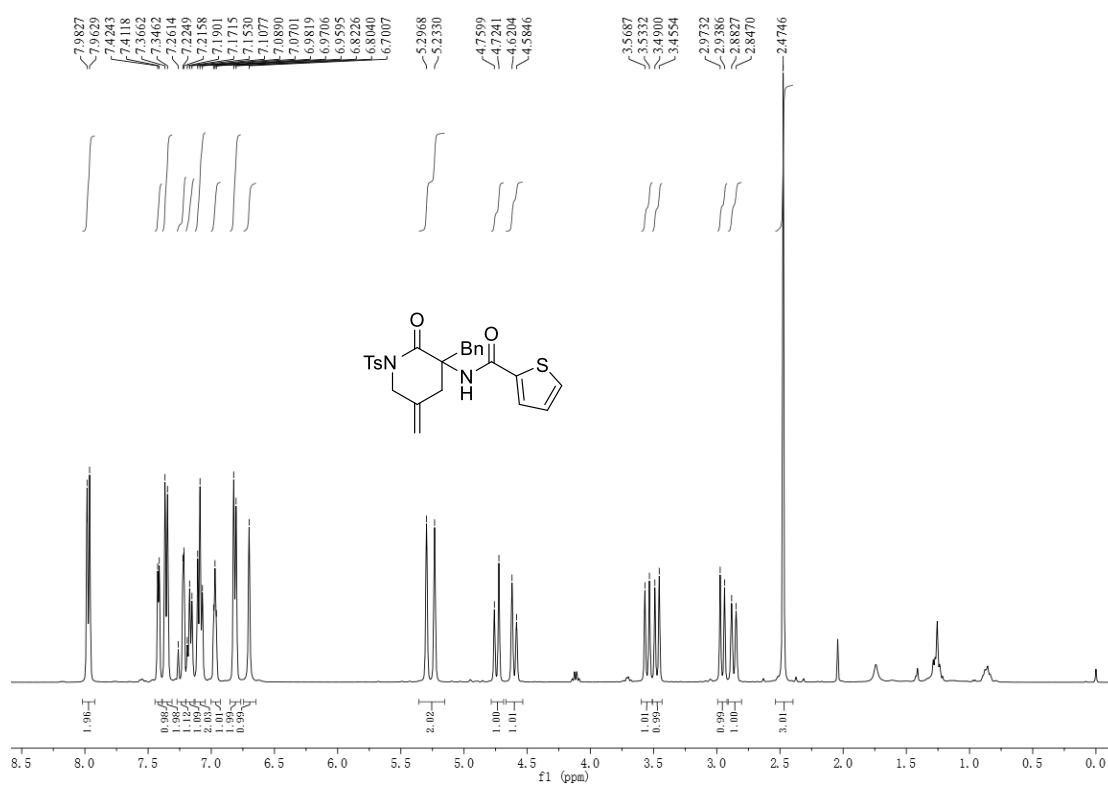
¹H and ¹³C NMR spectra for compound 5h



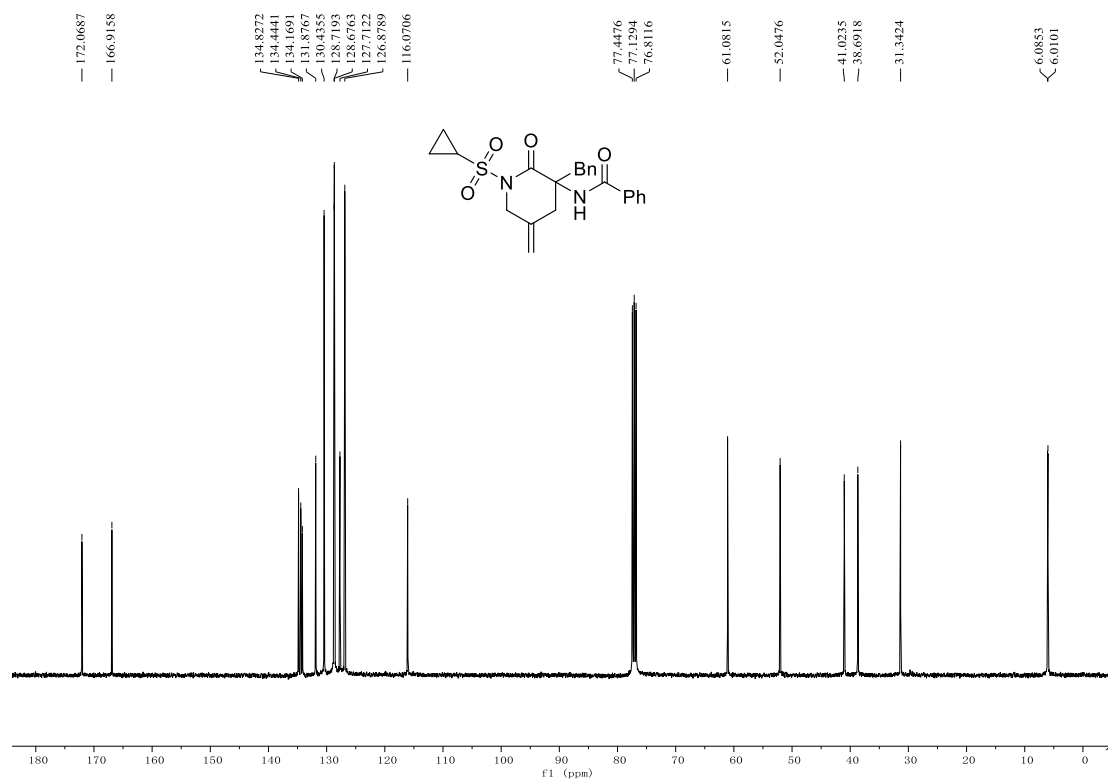
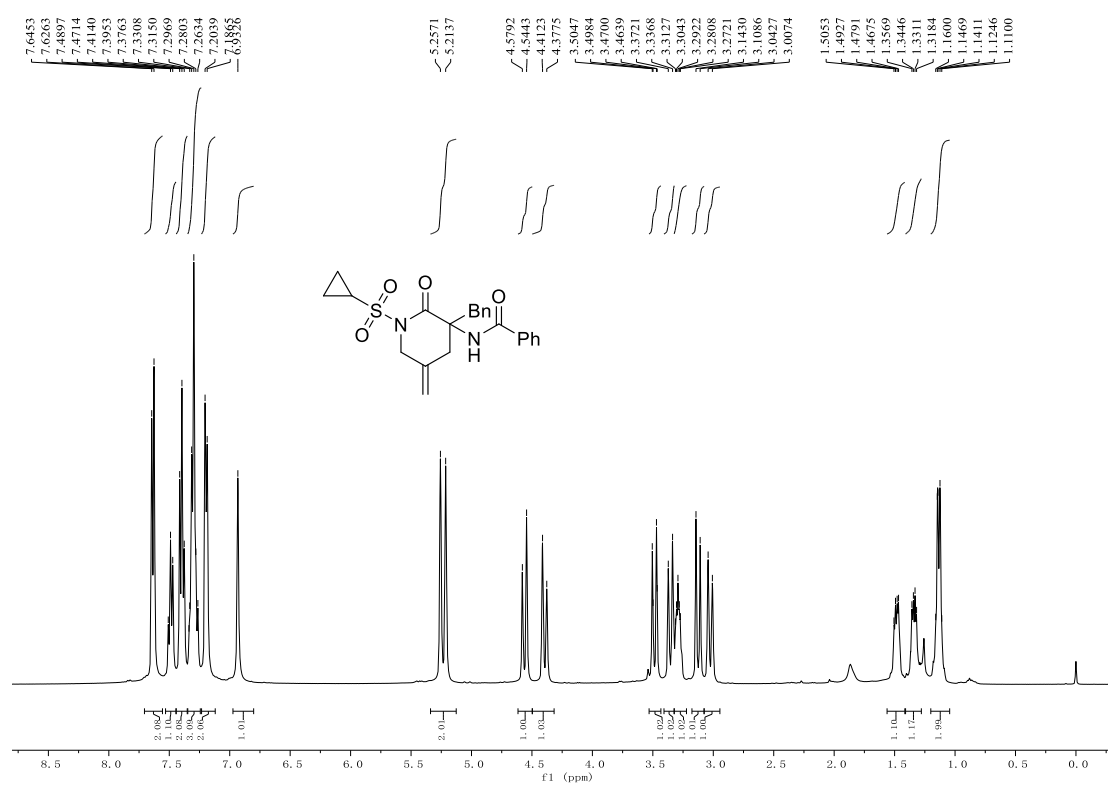
¹H and ¹³C NMR spectra for compound 5i



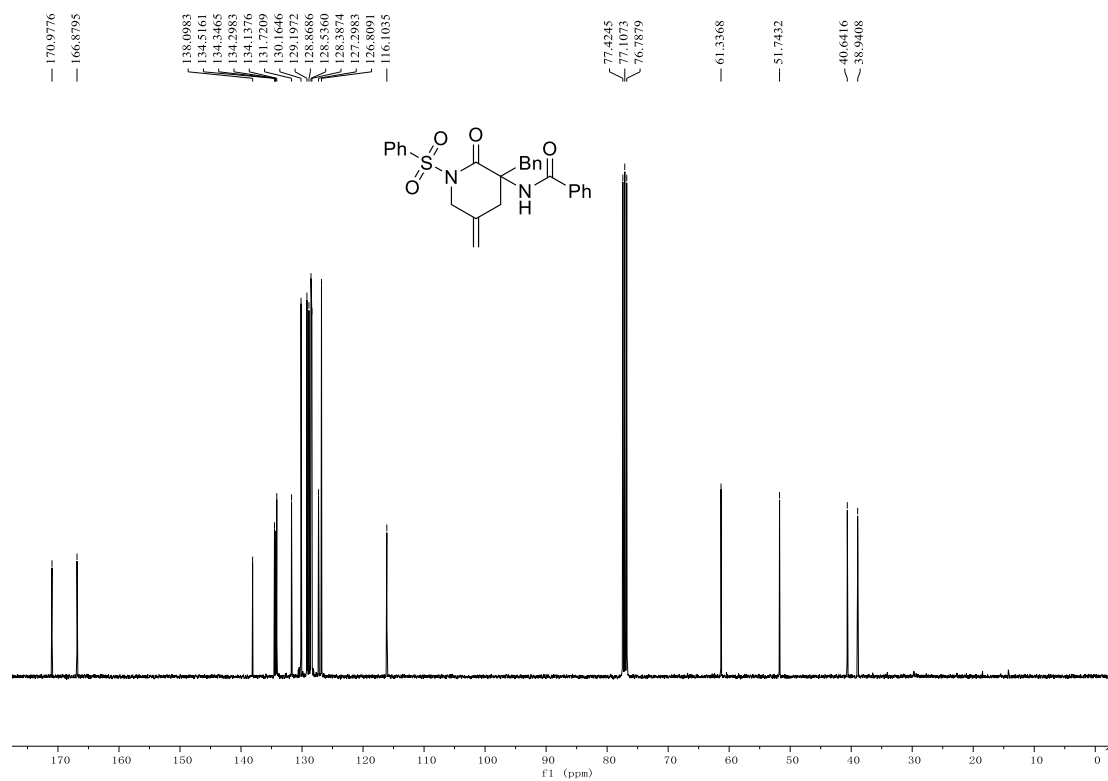
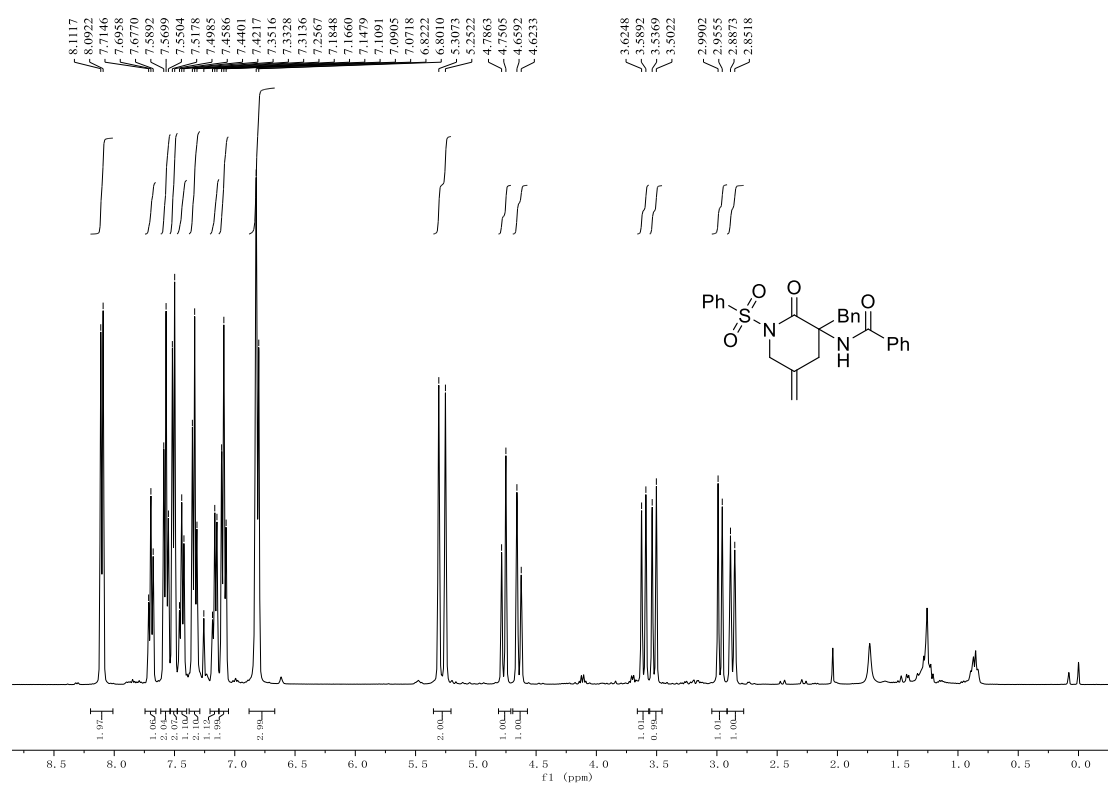
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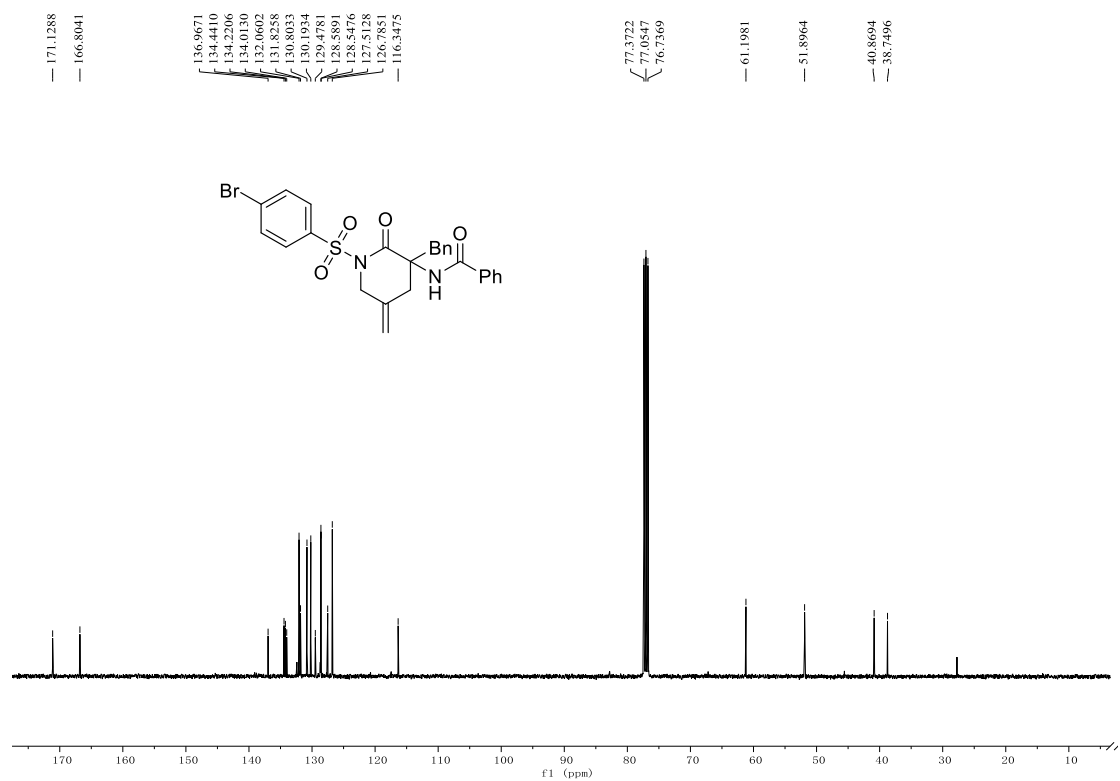
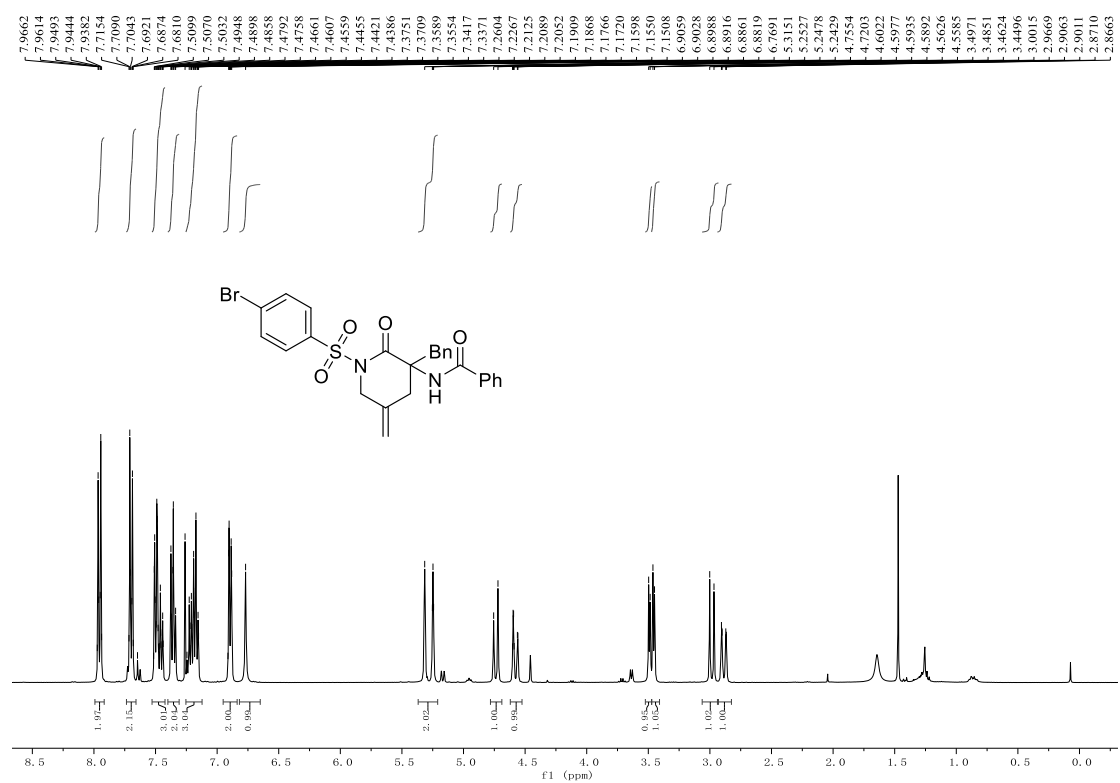
¹H and ¹³C NMR spectra for compound 5k



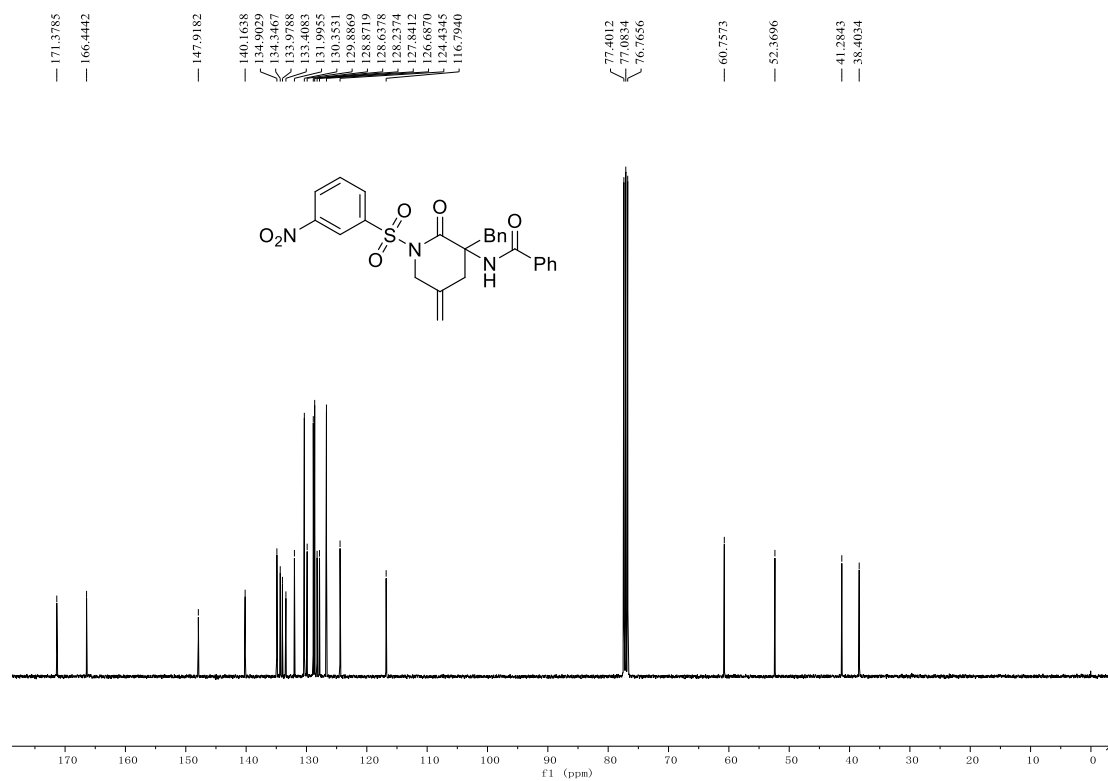
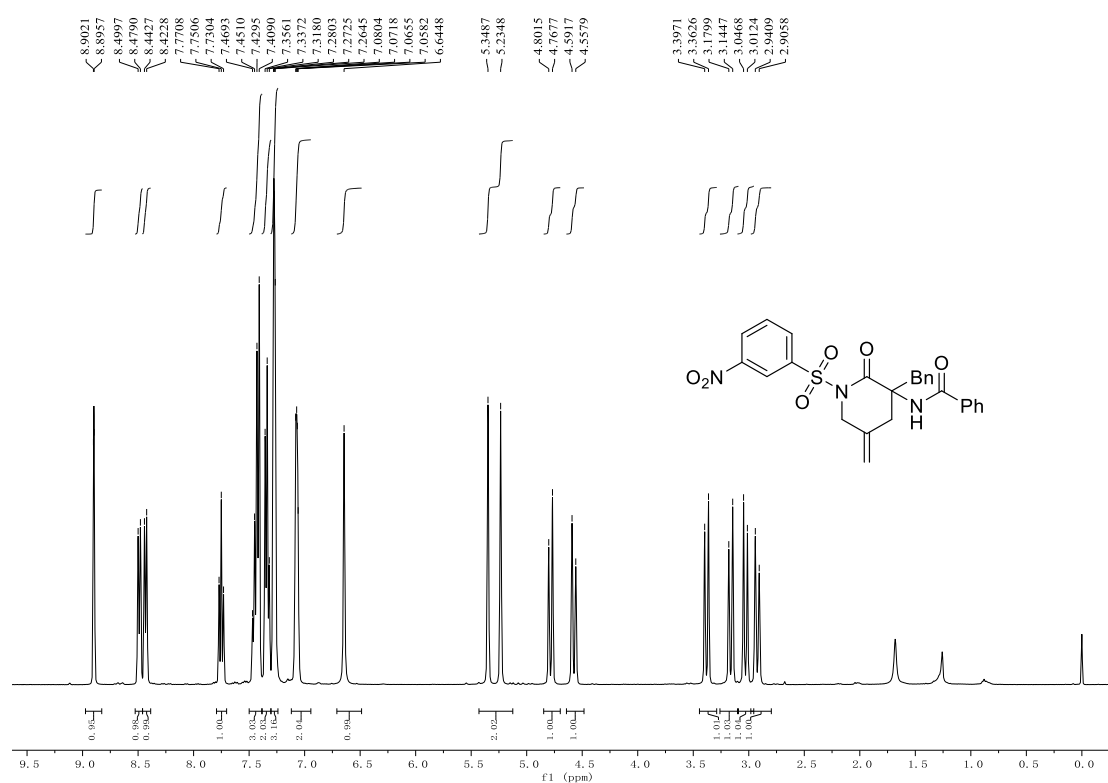
¹H and ¹³C NMR spectra for compound 5l



¹H and ¹³C NMR spectra for compound 5m



¹H and ¹³C NMR spectra for compound 5n



¹H and ¹³C NMR spectra for compound 6

