Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Ag_2CO_3/TFA Catalyzed Intramolecular Annulation Approach to Imidazo[1,2-*c*][1,3]oxazin-5-one Derivatives

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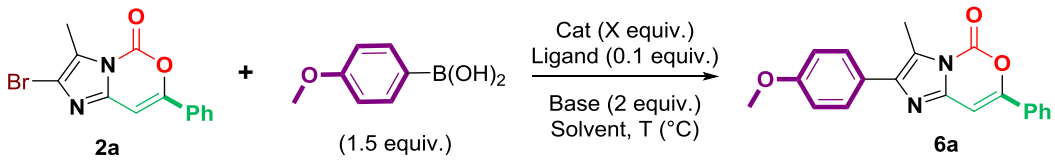
Contents:

1. Optimizations of Suzuki-Miyaura and Sonogashira cross-couplings at C-2 of **2a**

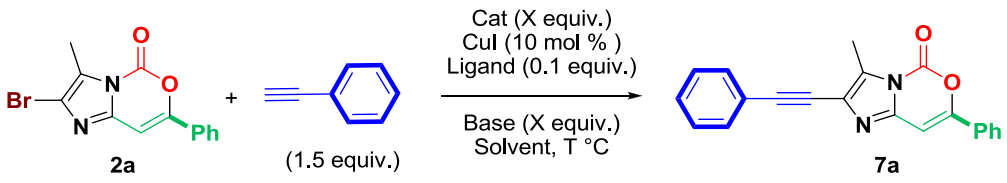
Table S1. Optimization of Suzuki-Miyaura cross-coupling between 2a and 4-methoxyphenylboronic acid.



Entry	Solvent	Catalyst (equiv.)	Base	Ligand	T (°C)	Time (h)	**6a/2a**
1	Dioxane/H_2O (4/1)	$PdCl_2dppf$ (0.1)	Na_2CO_3	-	65	1	-[b]
2	DME/EtOH/H_2O (3/1/1)	$Pd(OAc)_2$ (0.04)	Na_2CO_3	-	65[a]	1	-[b]
3	Toluène/MeOH (4/1)	$PdPPh_3$ (0.1)	Na_2CO_3	-	80	1	-[b]
4	Toluène/H_2O (5/0.5)	$PdCl_2(PPh_3)_2$ (0.1)	Na_2CO_3	-	80	1	-[b]
5	Toluène/H_2O (5/0.5)	$PdCl_2(PPh_3)_2$ (0.1)	K_3PO_4	-	80	24	6/94
6	Toluene/H_2O (5/0.5)	$Pd_2(dba)_3$ (0.025)	K_3PO_4	-	110	24	12/88
7	**Toluene/H_2O (5/0.5)**	**$Pd_2(dba)_3$ (0.025)**	**K_3PO_4**	**XPhos**	**110**	**1**	**100/0**
8	EtOH/H_2O (4/1)	$XPhosPdG_2$ (0.1)	K_2CO_3	Xphos	65[a]	1	-[b]

[a]Reaction was performed under microwave irradiation. [b]Degradation of the reaction.

Table S2. Optimization of Sonogashira cross-coupling between 2a and phenylacetylene.

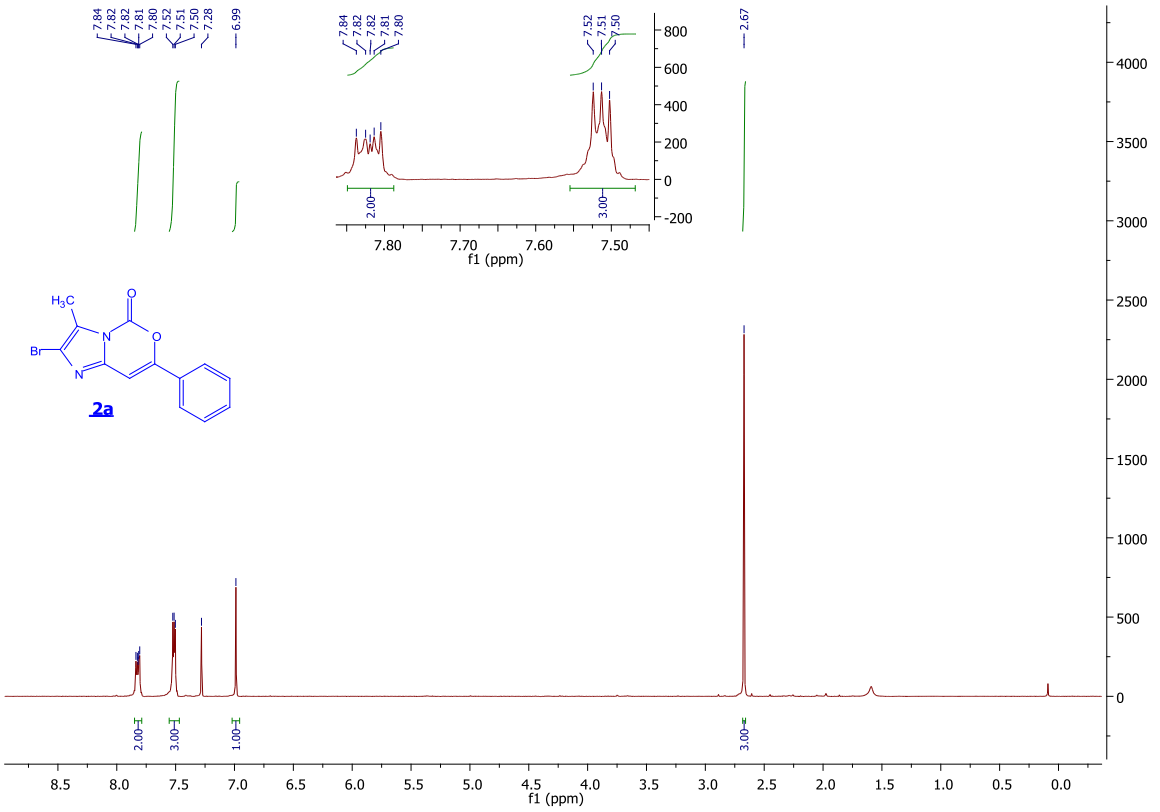


Entry	Solvent	Catalyst (equiv.)	Base (equiv.)	Ligand	T(°C)	Time (h)	**7a/2a**
1	Toluène	$PdCl_2(PPh_3)_2$ (0.1)	Et_3N (5.0)	PPh_3	110	48	0/100
2	Et_3N	$PdCl_2(PPh_3)_2$ (0.1)	--	--	110	48	0/100
3	Et_3N	$PdCl_2(PPh_3)_2$ (0.1)	--	$AsPh_3$	110	48	0/100
4	**Et_3N**	**$Pd_2(dba)_3$ (0.05)**	**--**	**XPhos**	**80**	**1**	**100/0**
5[a]	DME/EtOH/H_2O (3/1/1)	$Pd(OAc)_2$ (0.04)	Et_3N (2.0)	PPh_3	70	1	-[b]

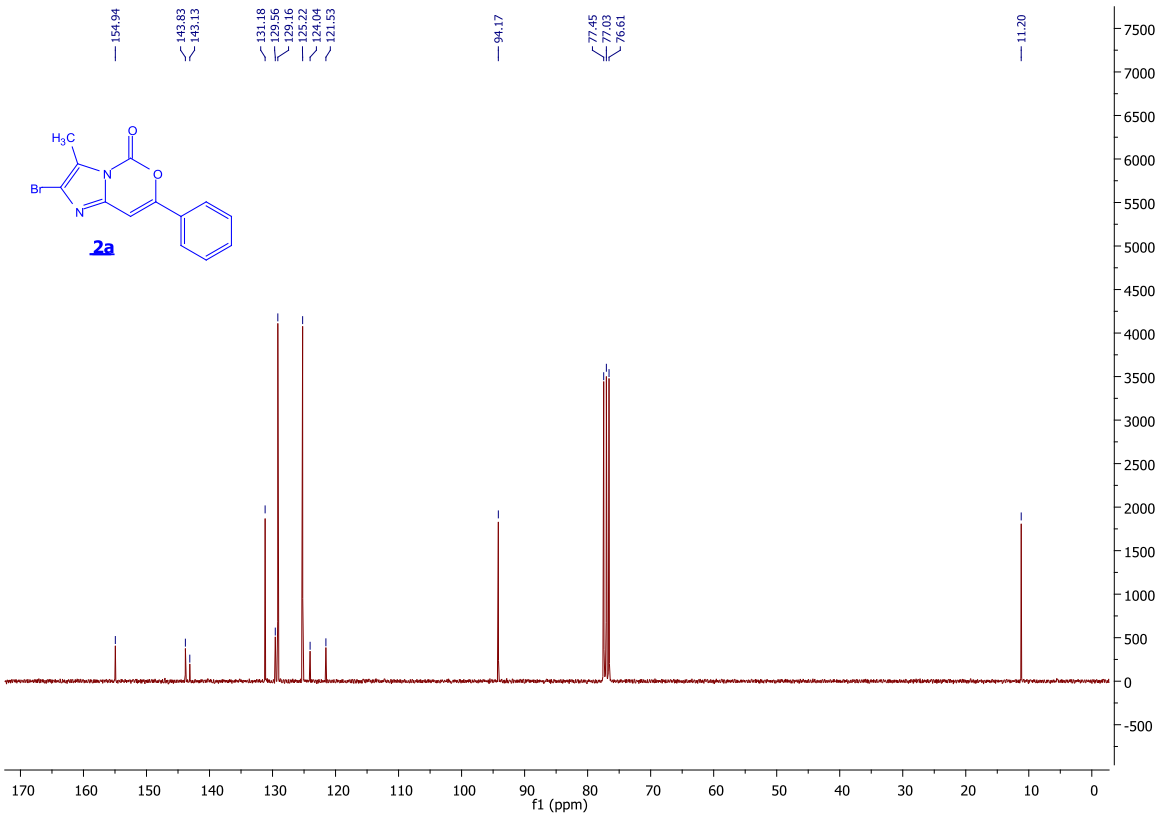
[a]Reaction carried out under microwave irradiation. [b]Degradation of the reaction

2. ^{1}H and ^{13}C NMR spectra of products

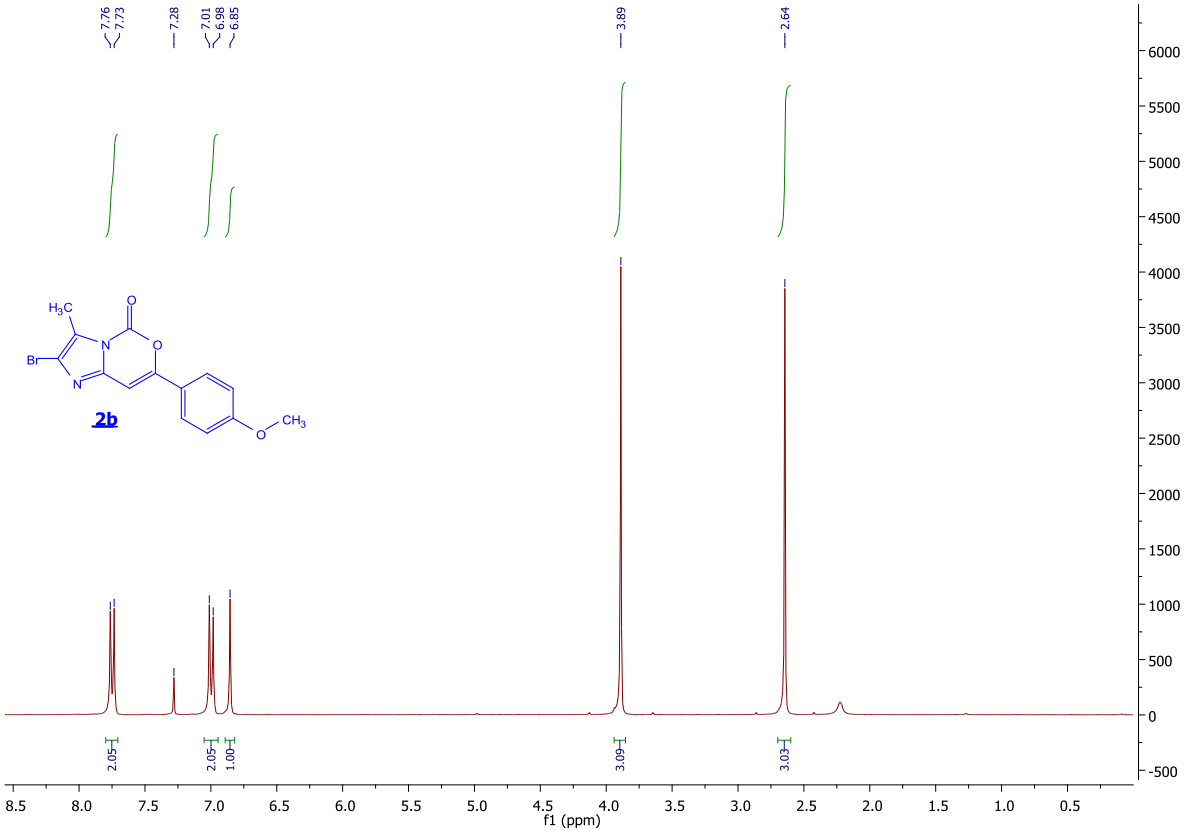
^{1}H NMR (300 MHz, $CDCl_3$) of **2a**



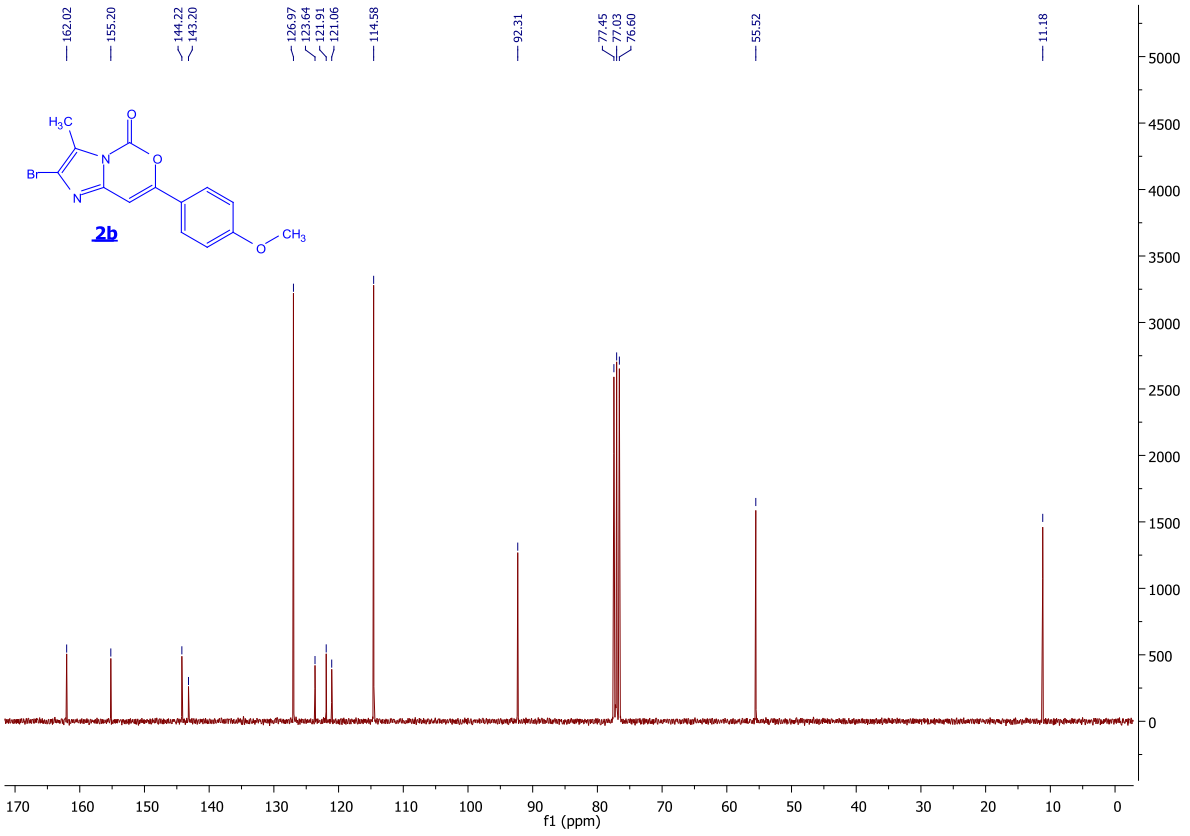
^{13}C NMR (75 MHz, $CDCl_3$) of **2a**



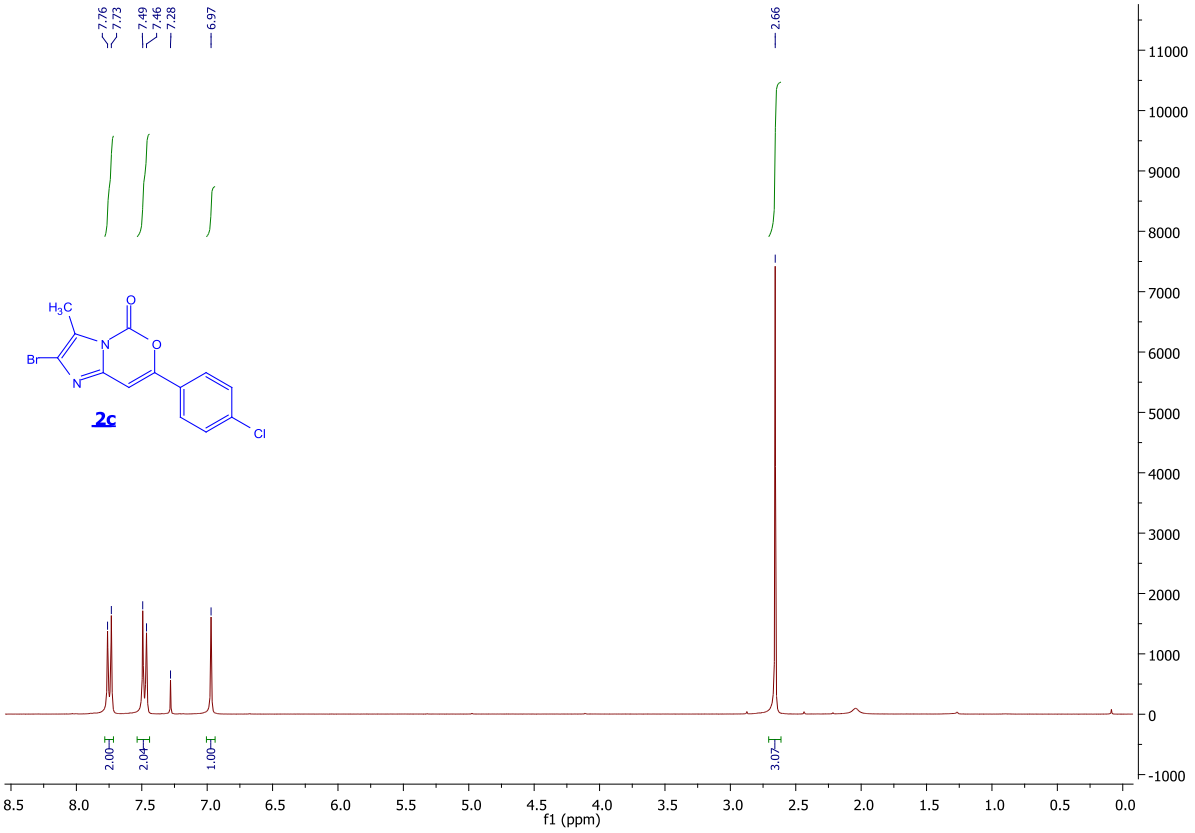
^{1}H NMR (300 MHz, $CDCl_3$) of **2b**



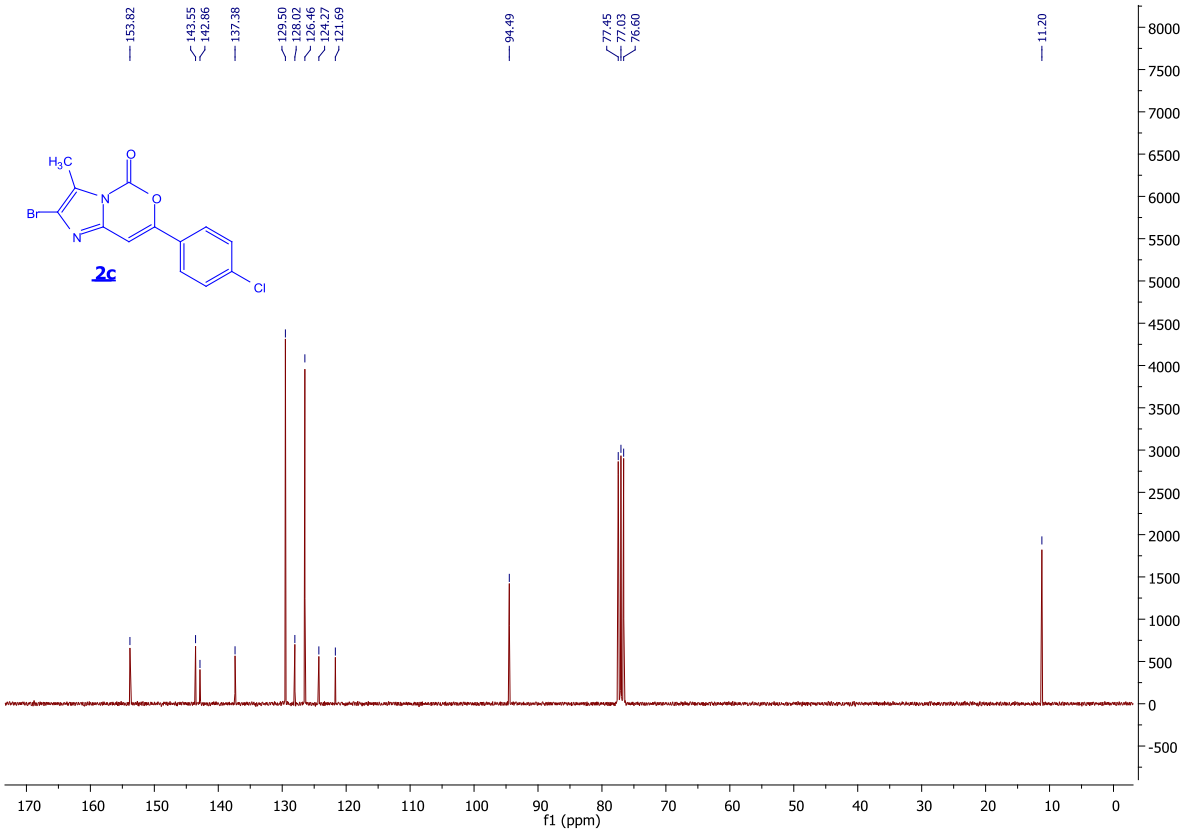
^{13}C NMR (75 MHz, $CDCl_3$) of **2b**



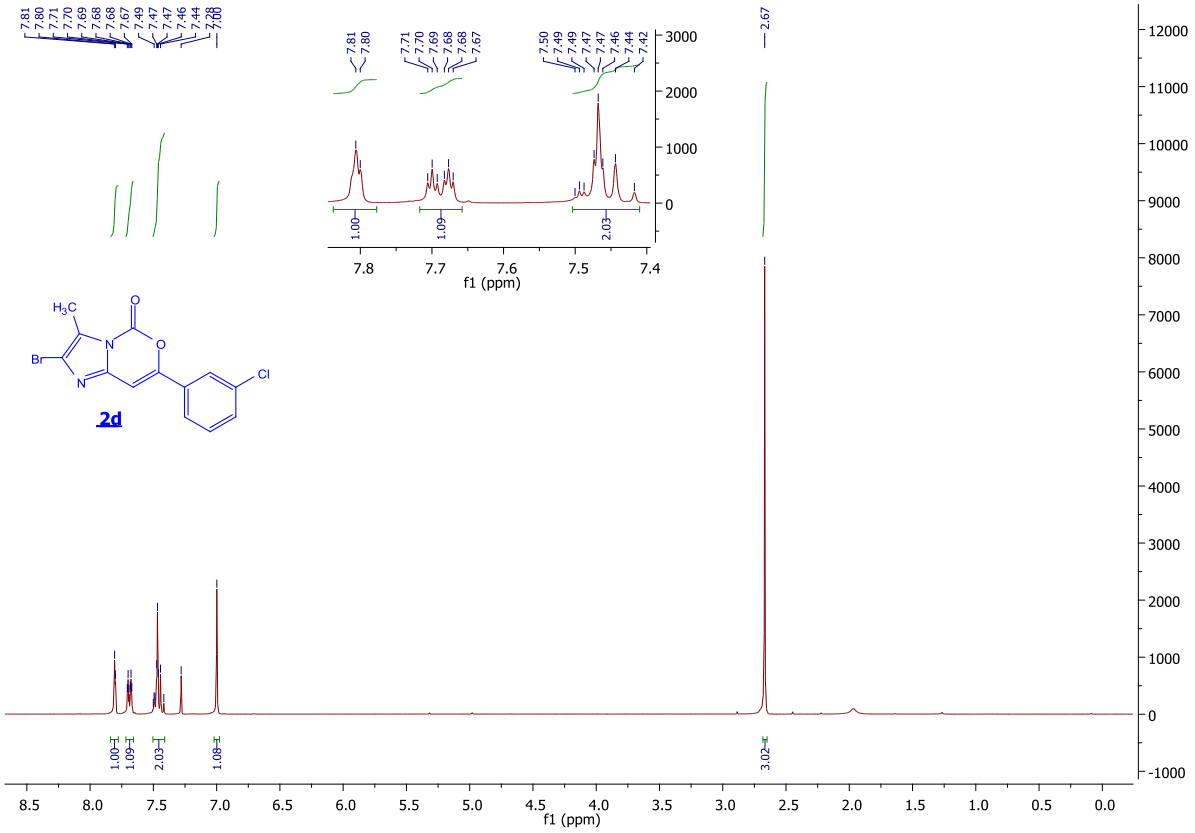
^{1}H NMR (300 MHz, $CDCl_3$) of **2c**



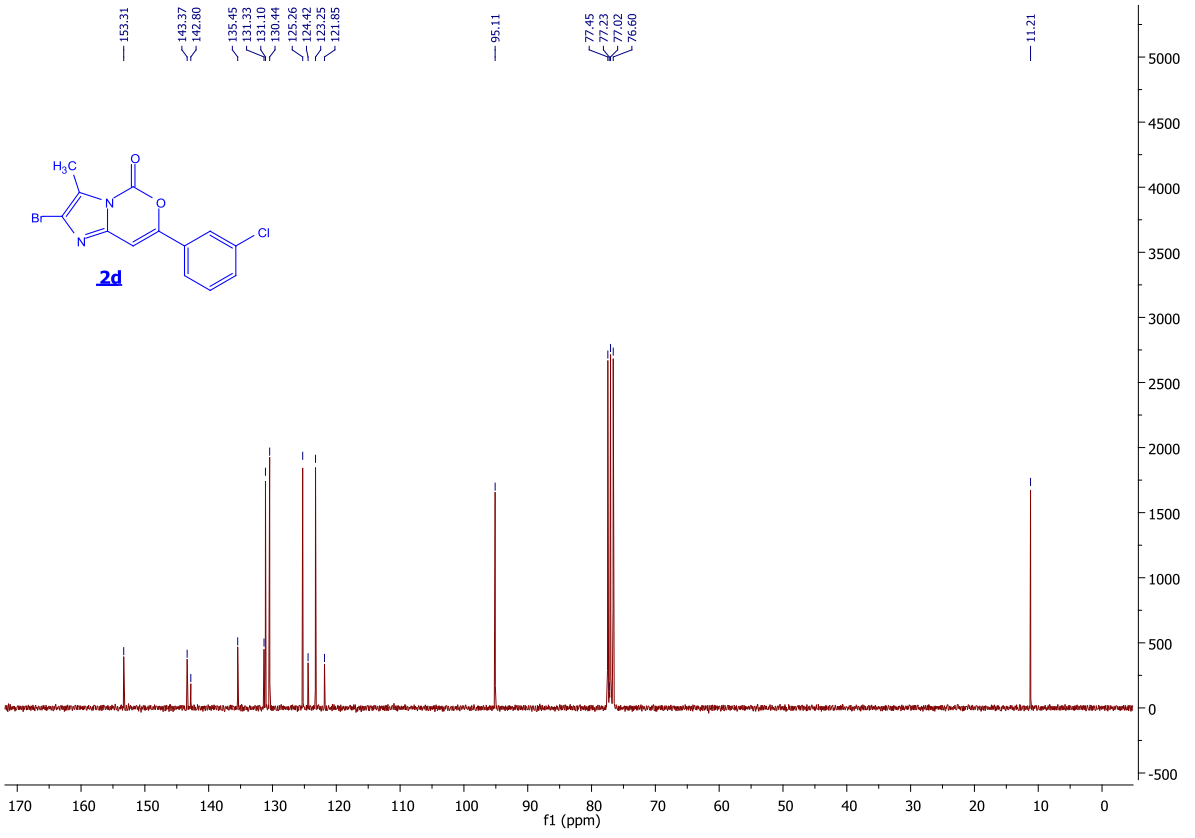
^{13}C NMR (75 MHz, $CDCl_3$) of **2c**



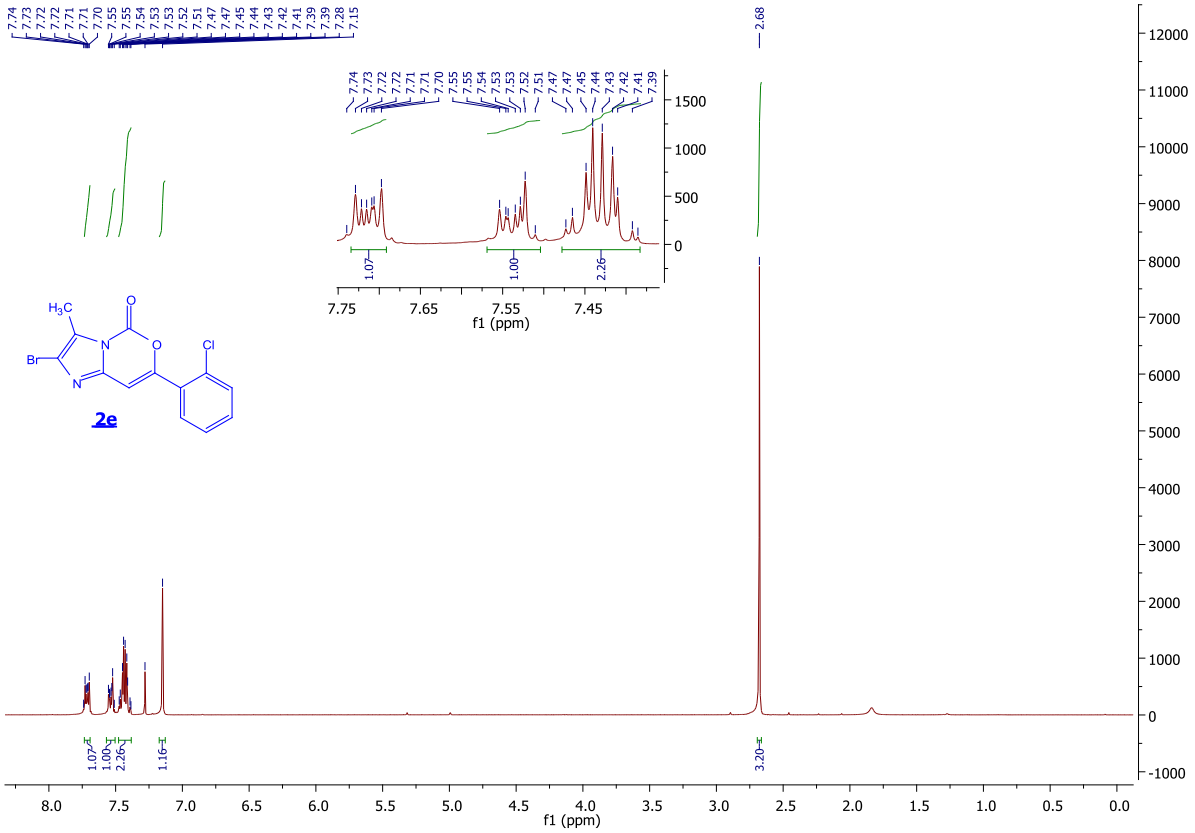
^{1}H NMR (300 MHz, $CDCl_3$) of **2d**



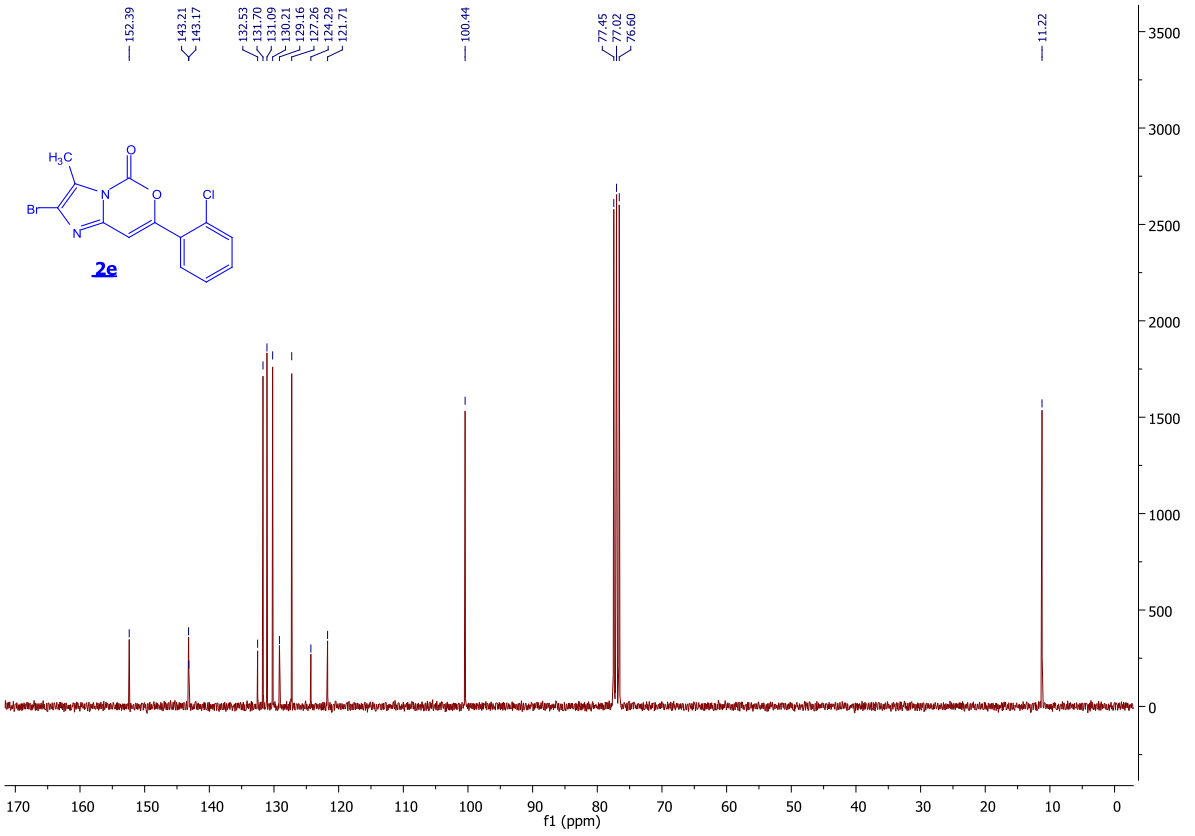
^{13}C NMR (75 MHz, $CDCl_3$) of **2d**



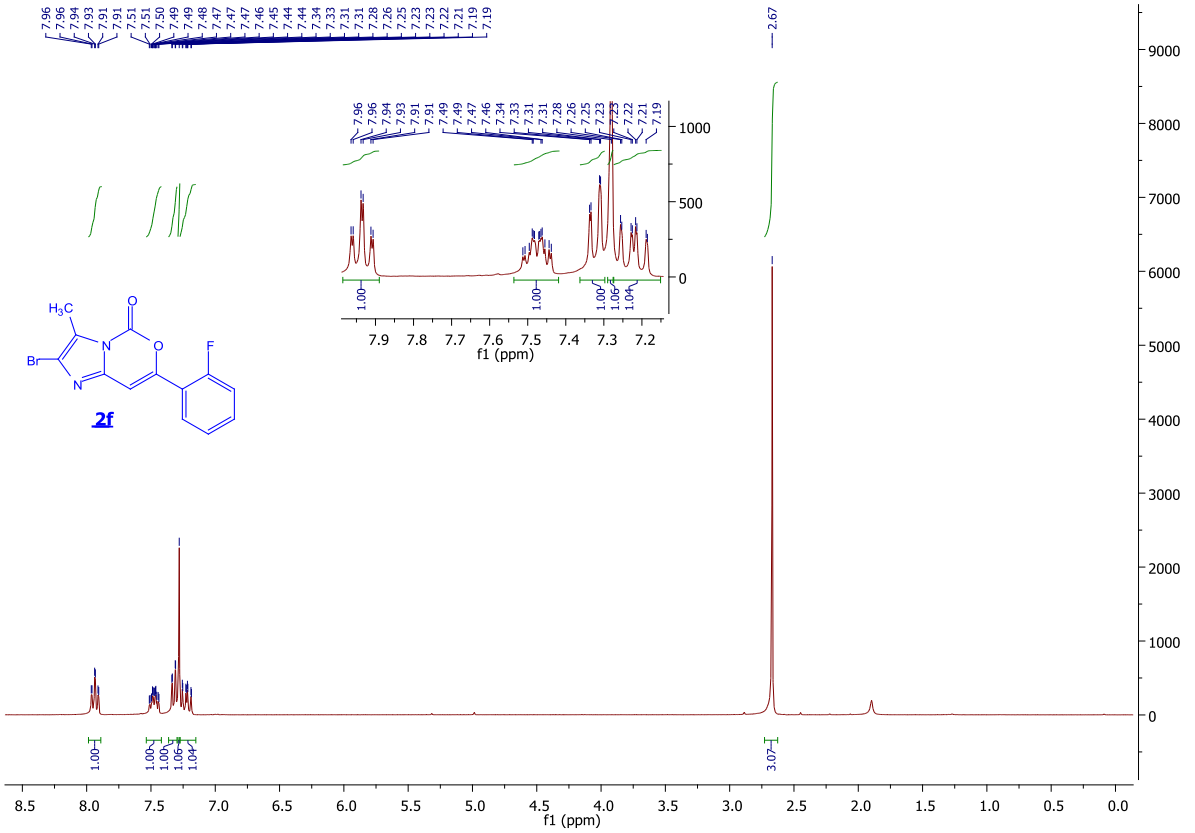
^{1}H NMR (300 MHz, $CDCl_3$) of **2e**



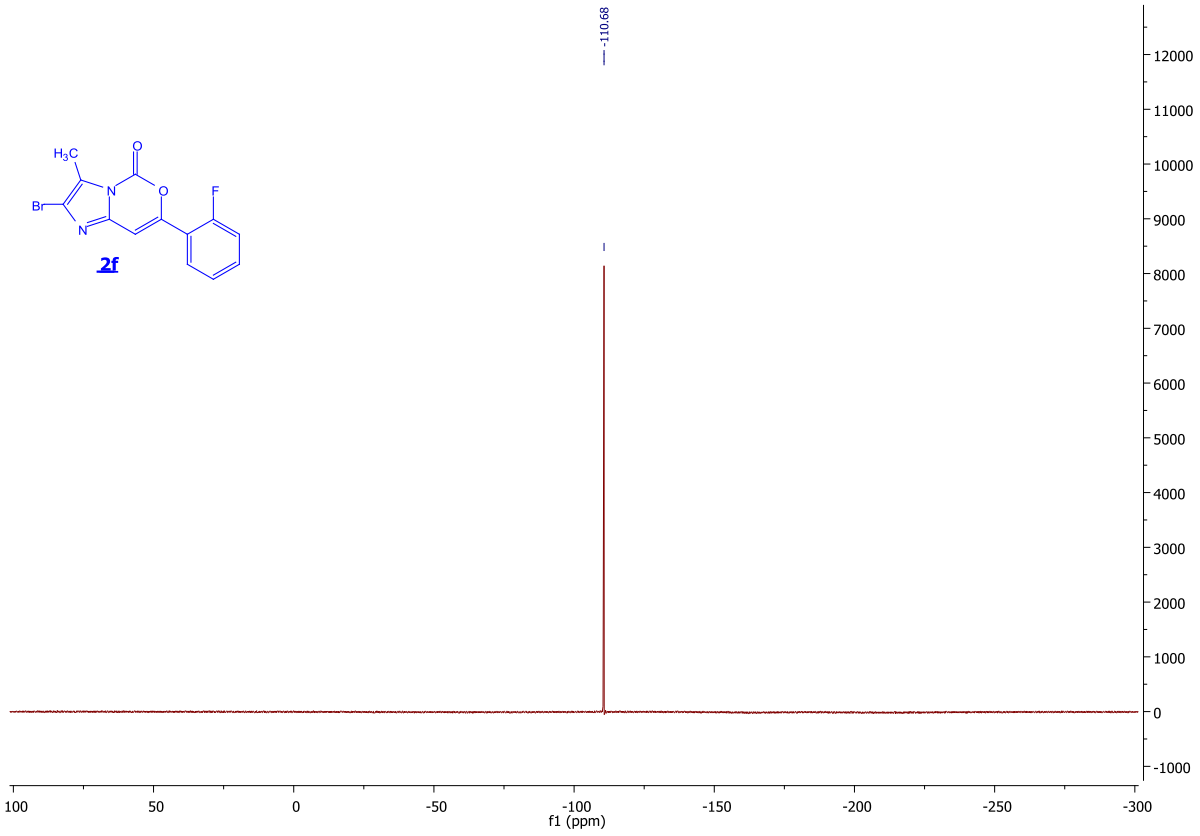
^{13}C NMR (75 MHz, $CDCl_3$) of **2e**



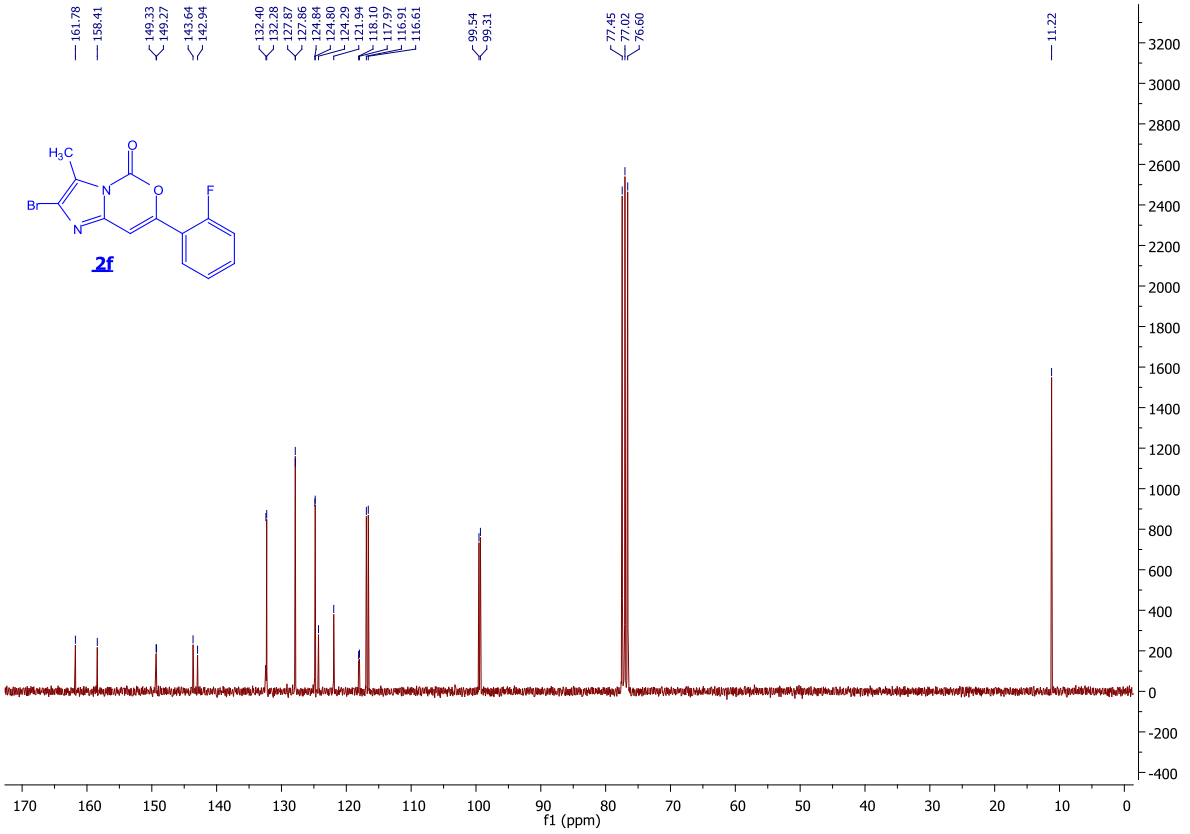
^{1}H NMR (300 MHz, $CDCl_3$) of **2f**



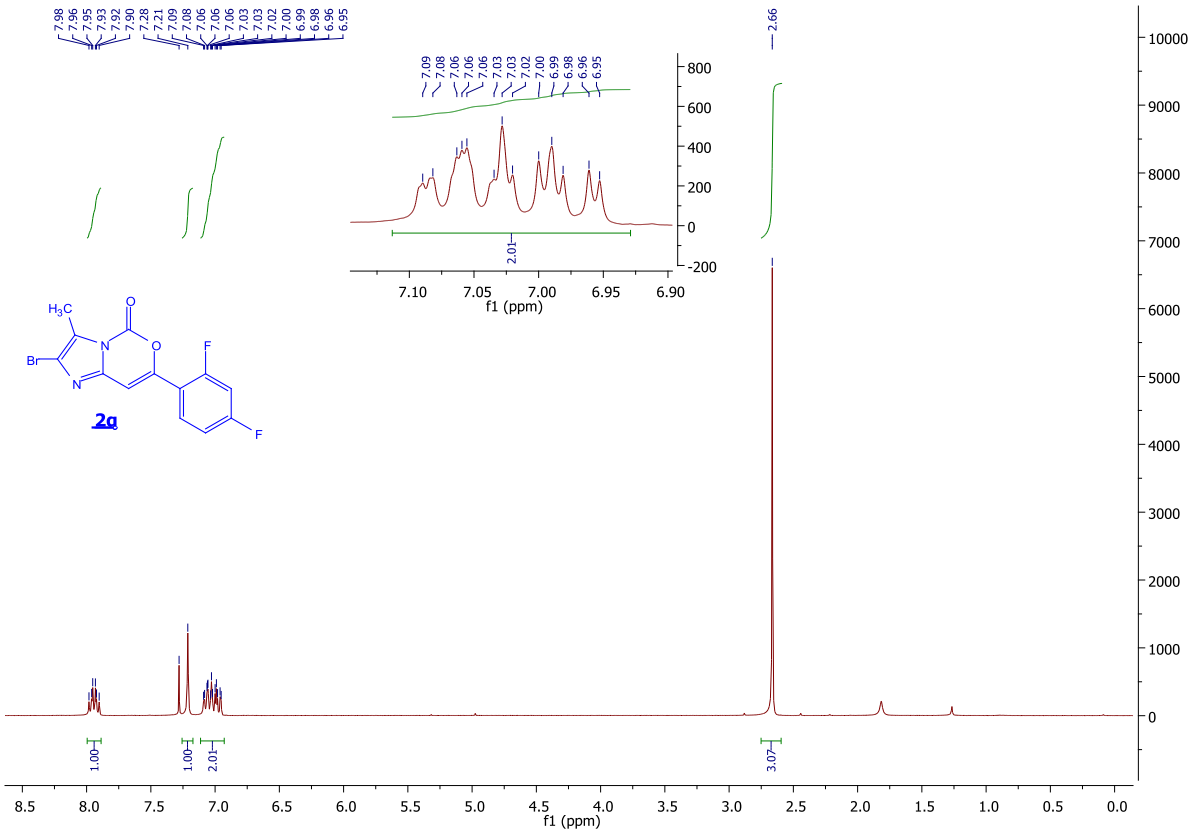
^{19}F NMR (282 MHz, $CDCl_3$) of **2f**



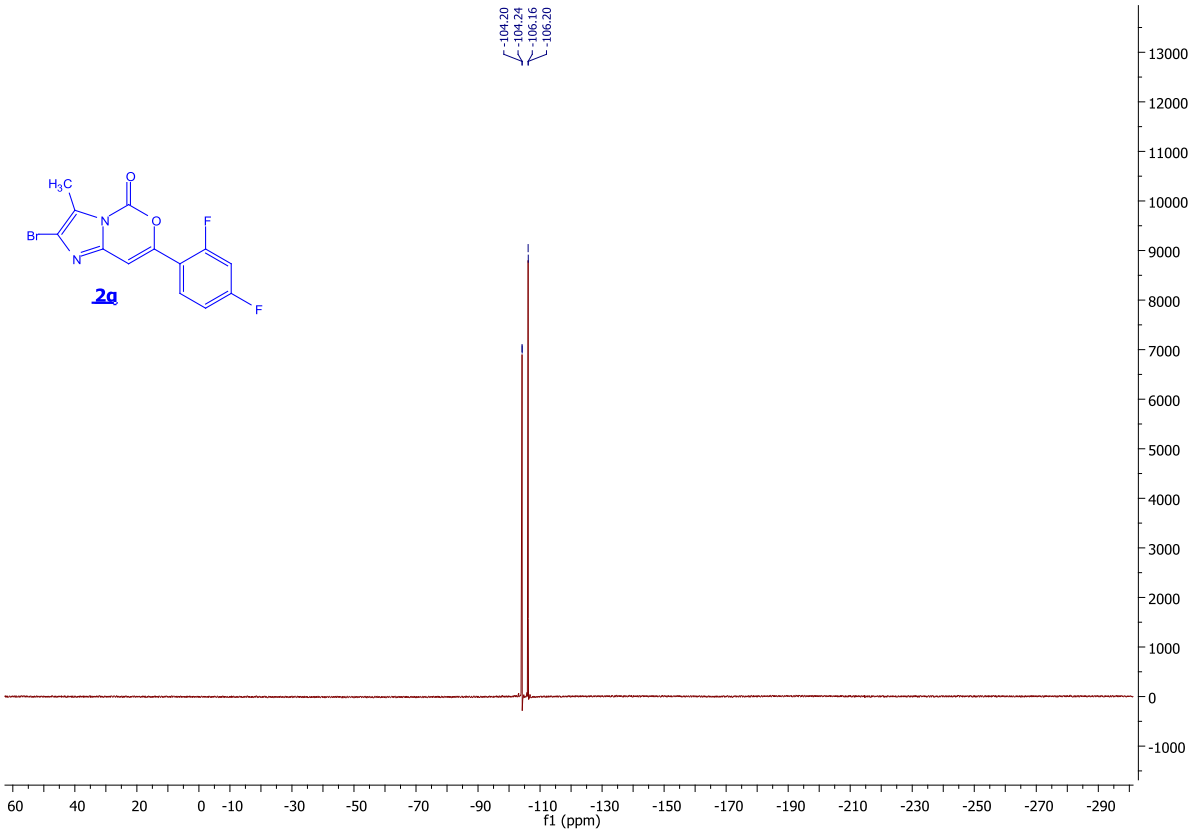
^{13}C NMR (75 MHz, $CDCl_3$) of **2f**



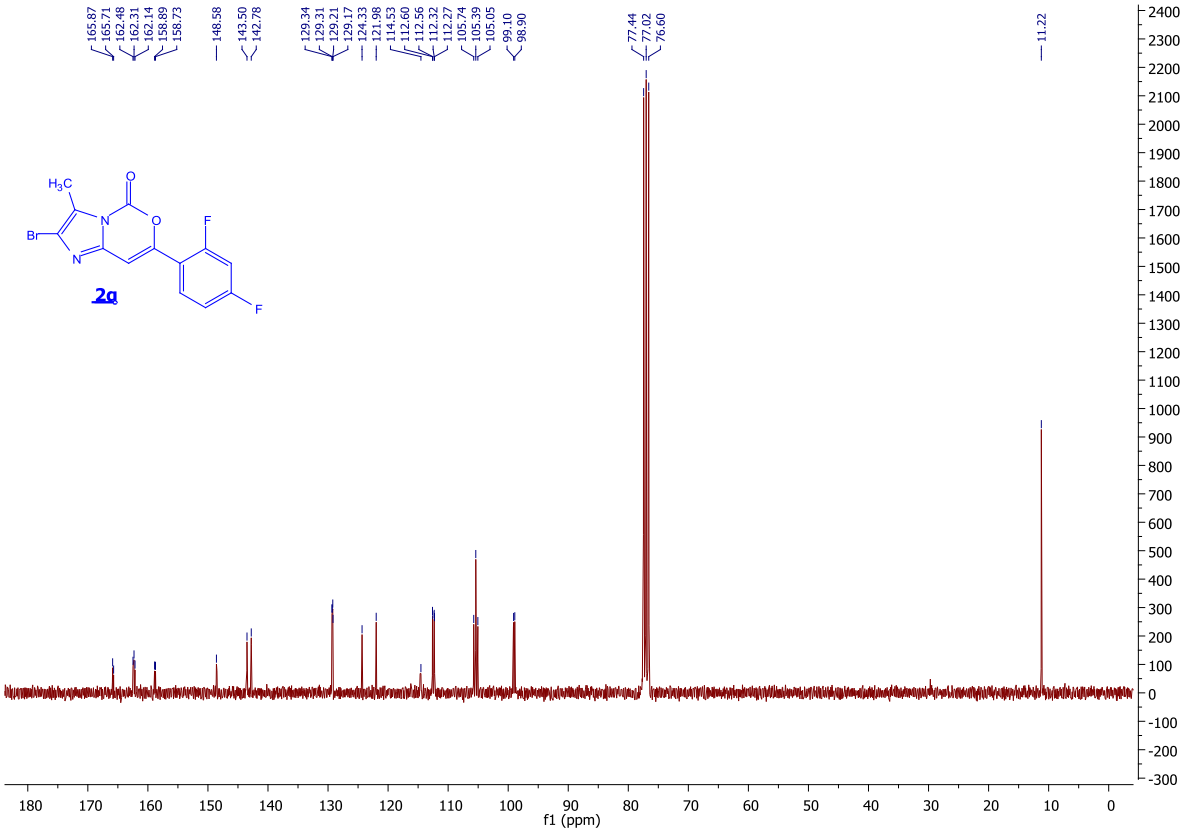
^{1}H NMR (300 MHz, $CDCl_3$) of **2g**



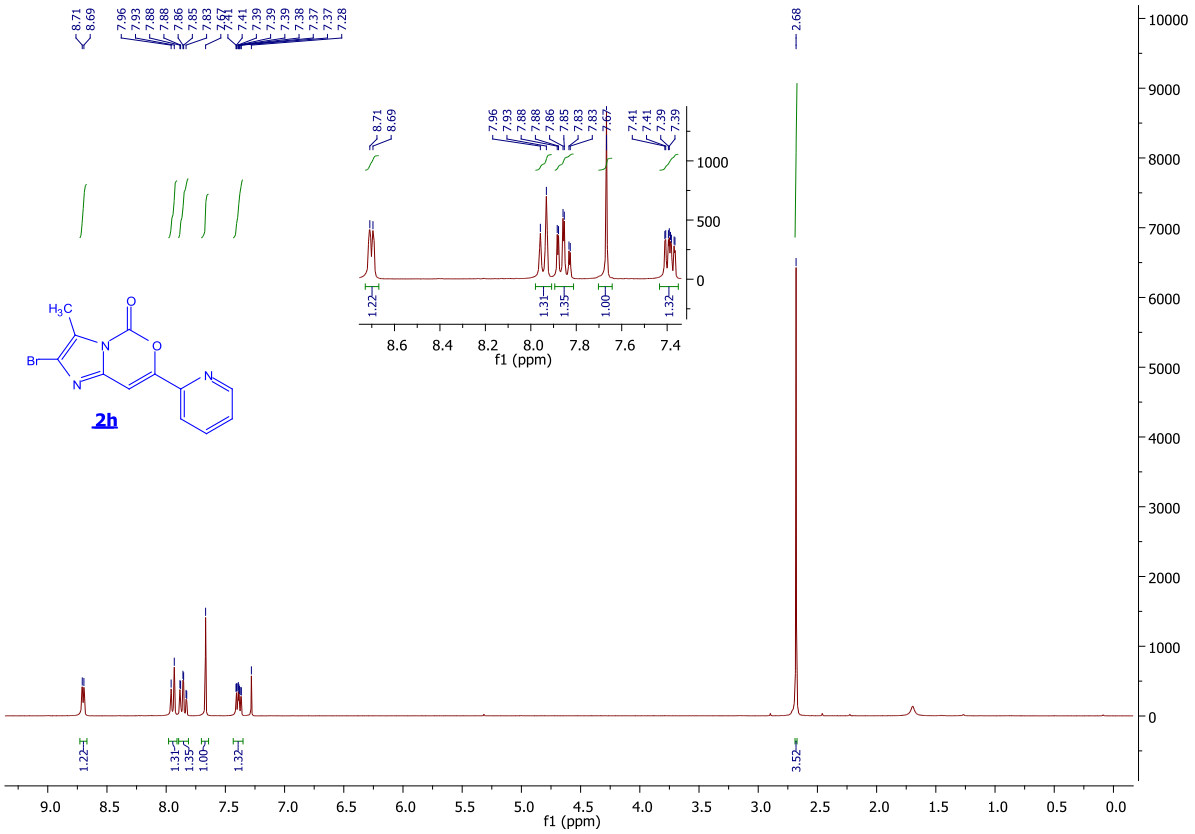
^{19}F NMR (282 MHz, $CDCl_3$) of **2g**



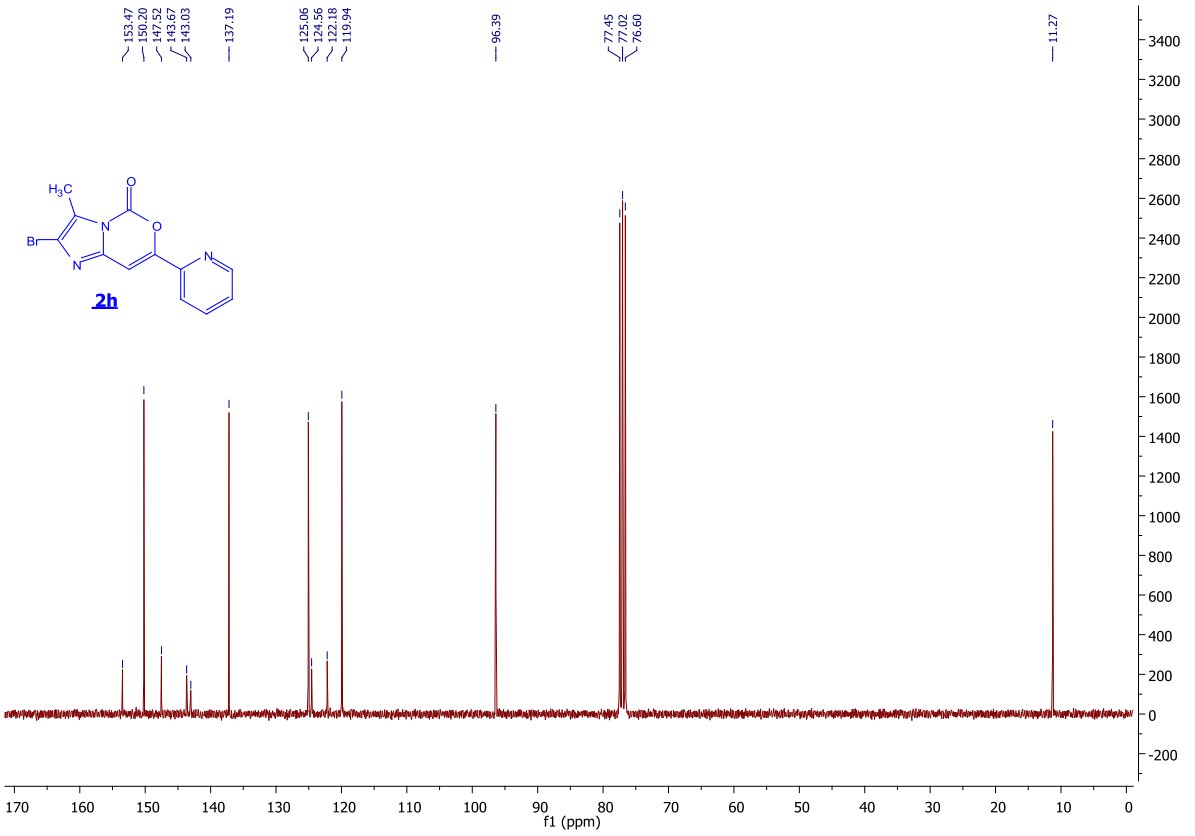
^{13}C NMR (75 MHz, $CDCl_3$) of **2g**



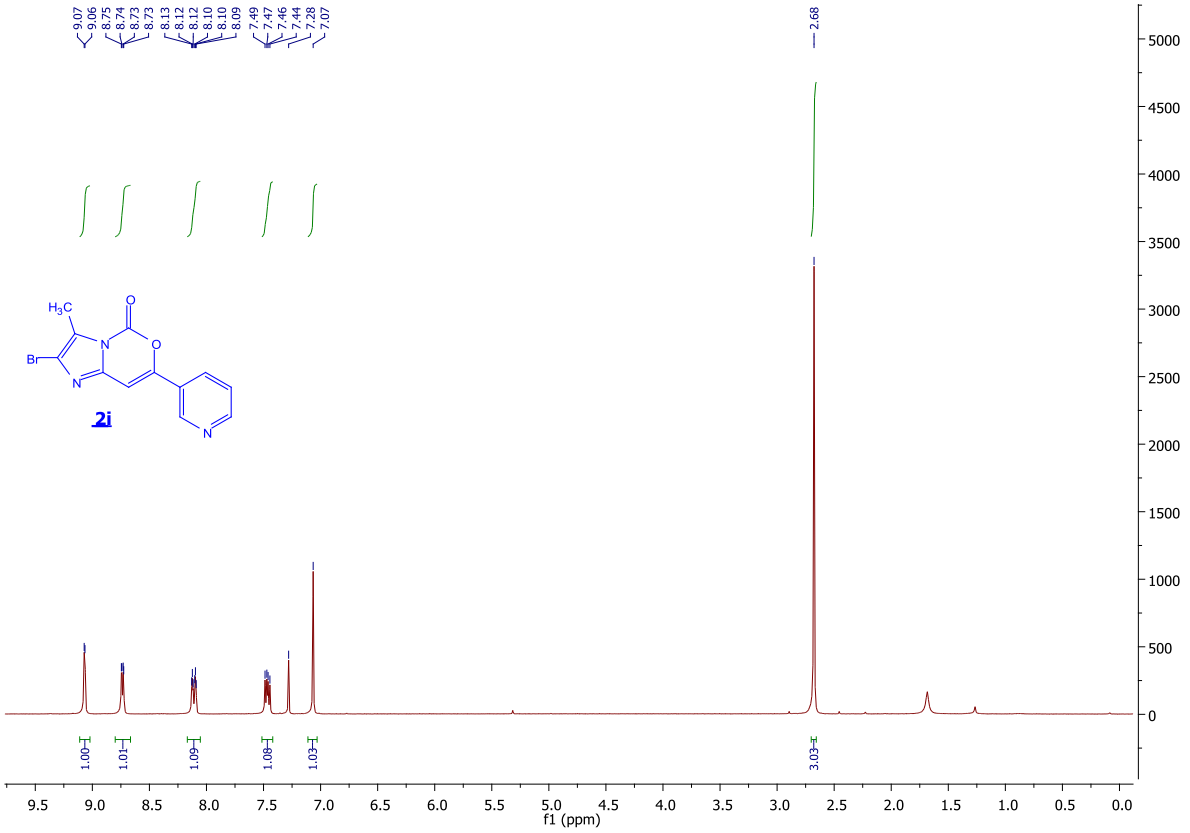
^{1}H NMR (300 MHz, $CDCl_3$) of **2h**



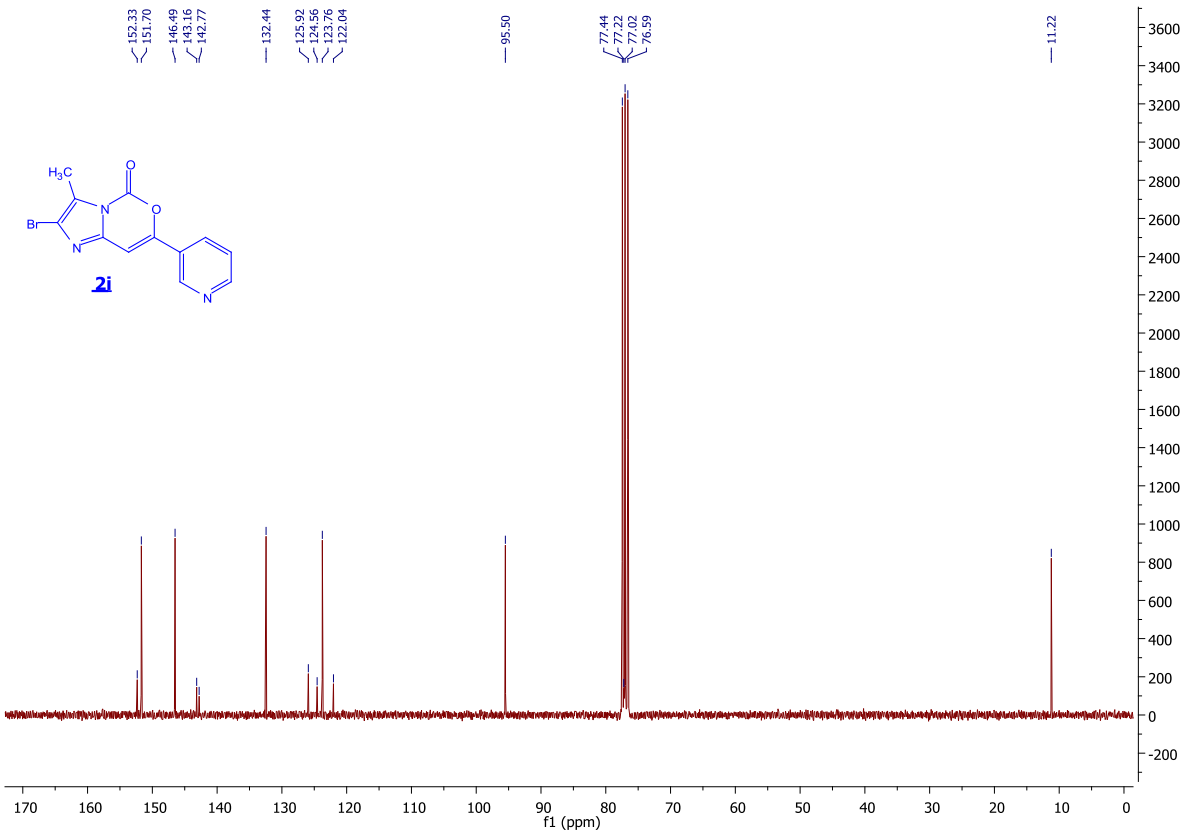
^{13}C NMR (75 MHz, $CDCl_3$) of **2h**



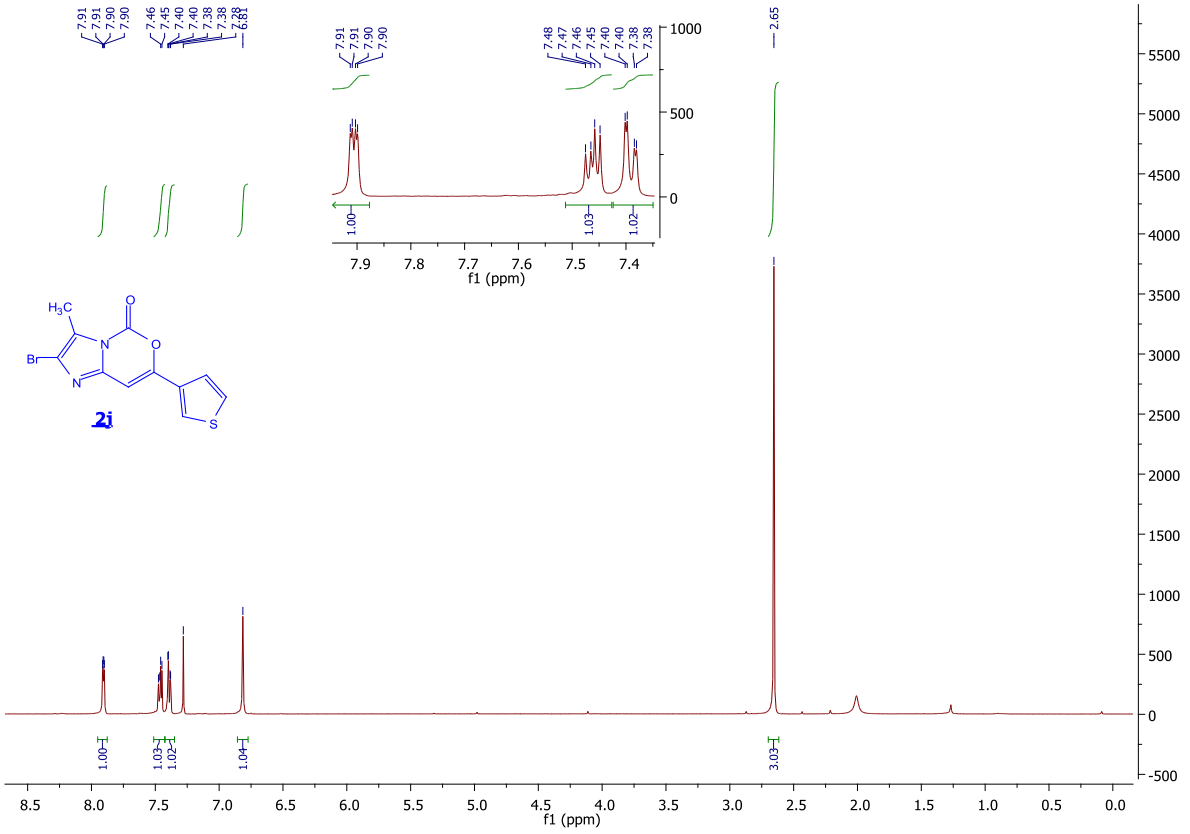
^{1}H NMR (300 MHz, $CDCl_3$) of **2i**



^{13}C NMR (75 MHz, $CDCl_3$) of **2i**



^{1}H NMR (300 MHz, $CDCl_3$) of **2j**



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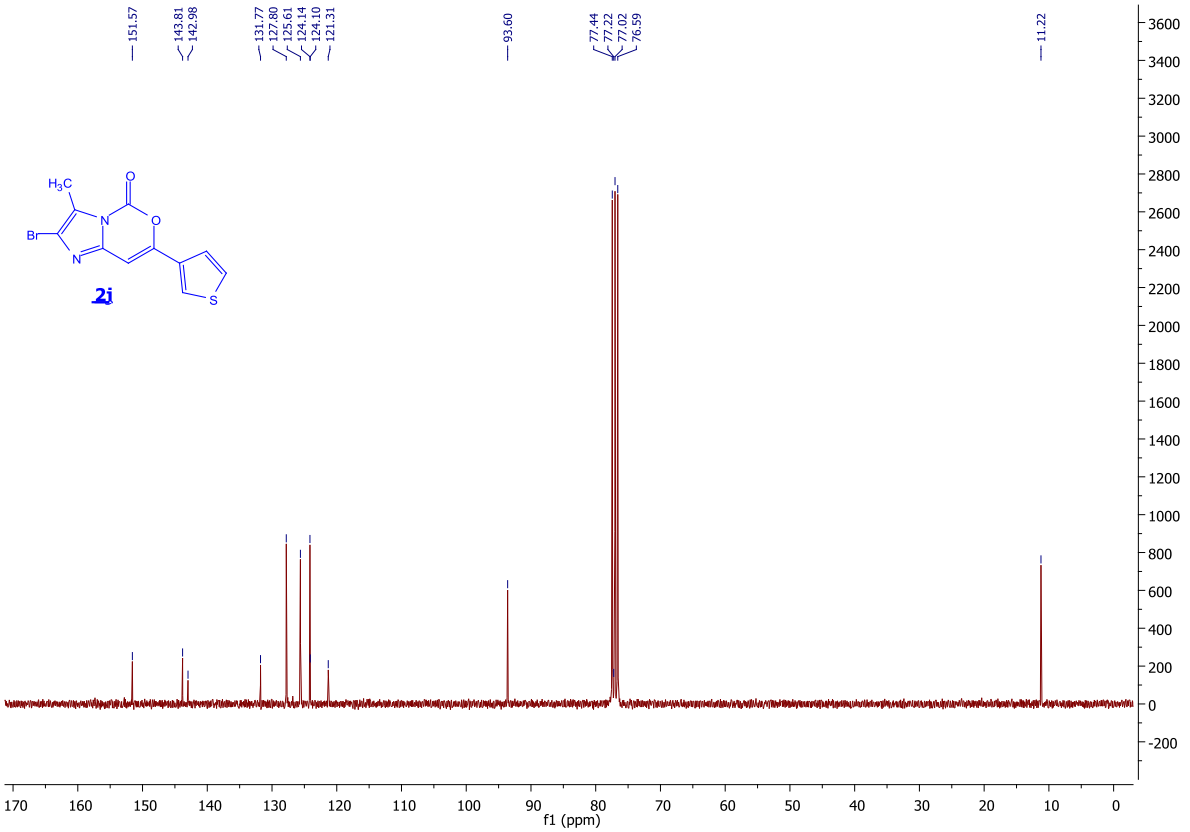
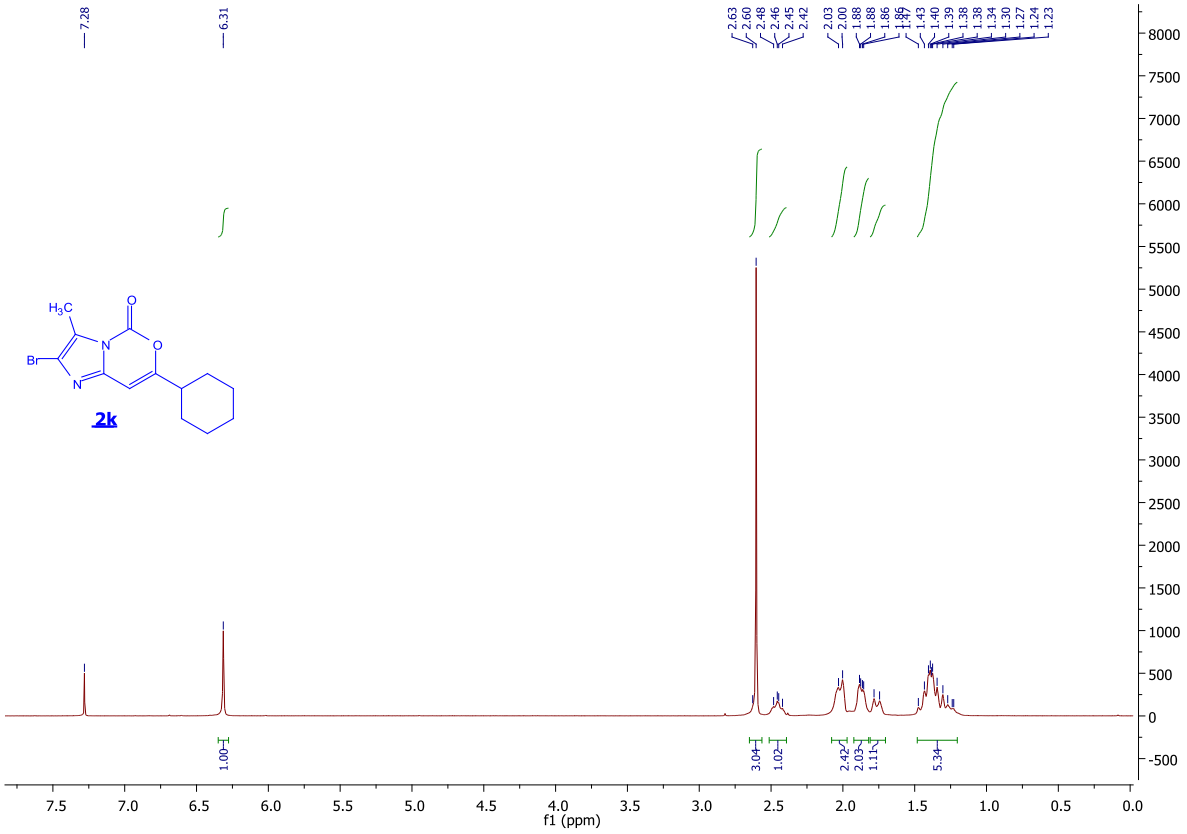


^{1}H NMR (300 MHz, $CDCl_3$) of **2k**



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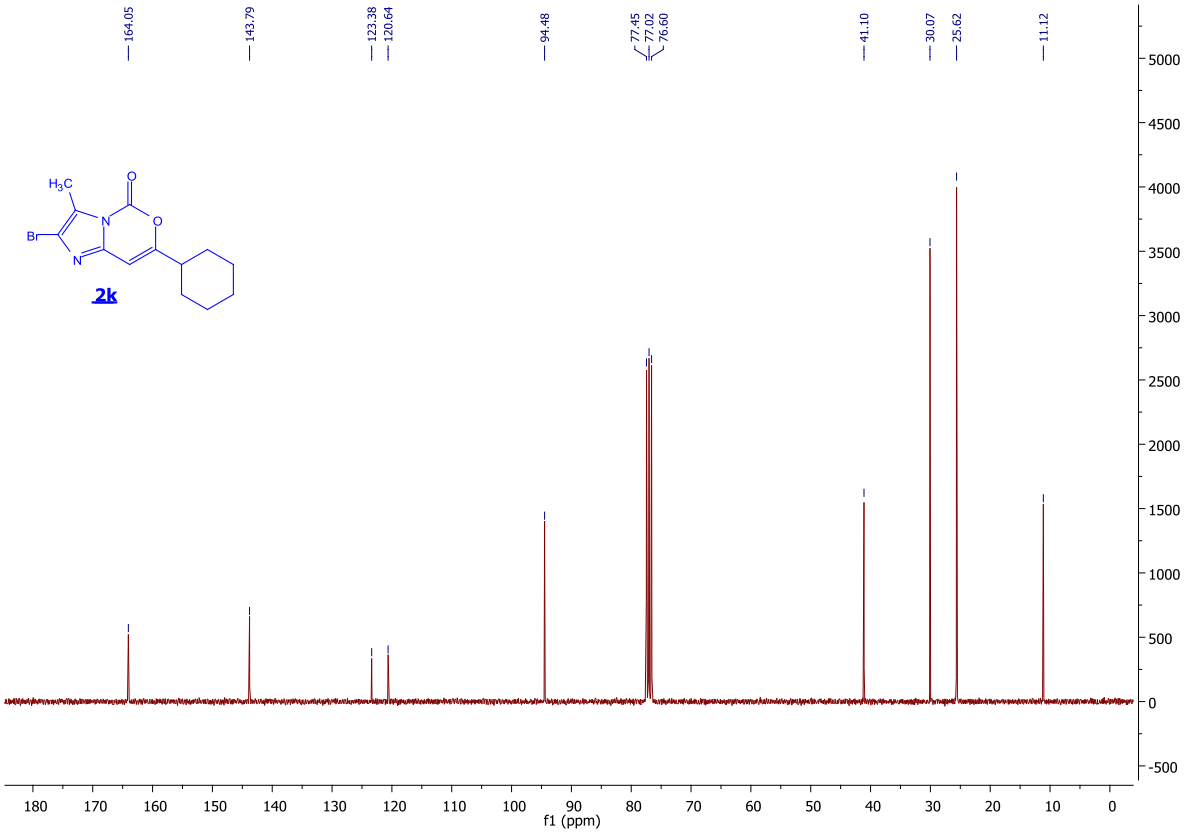

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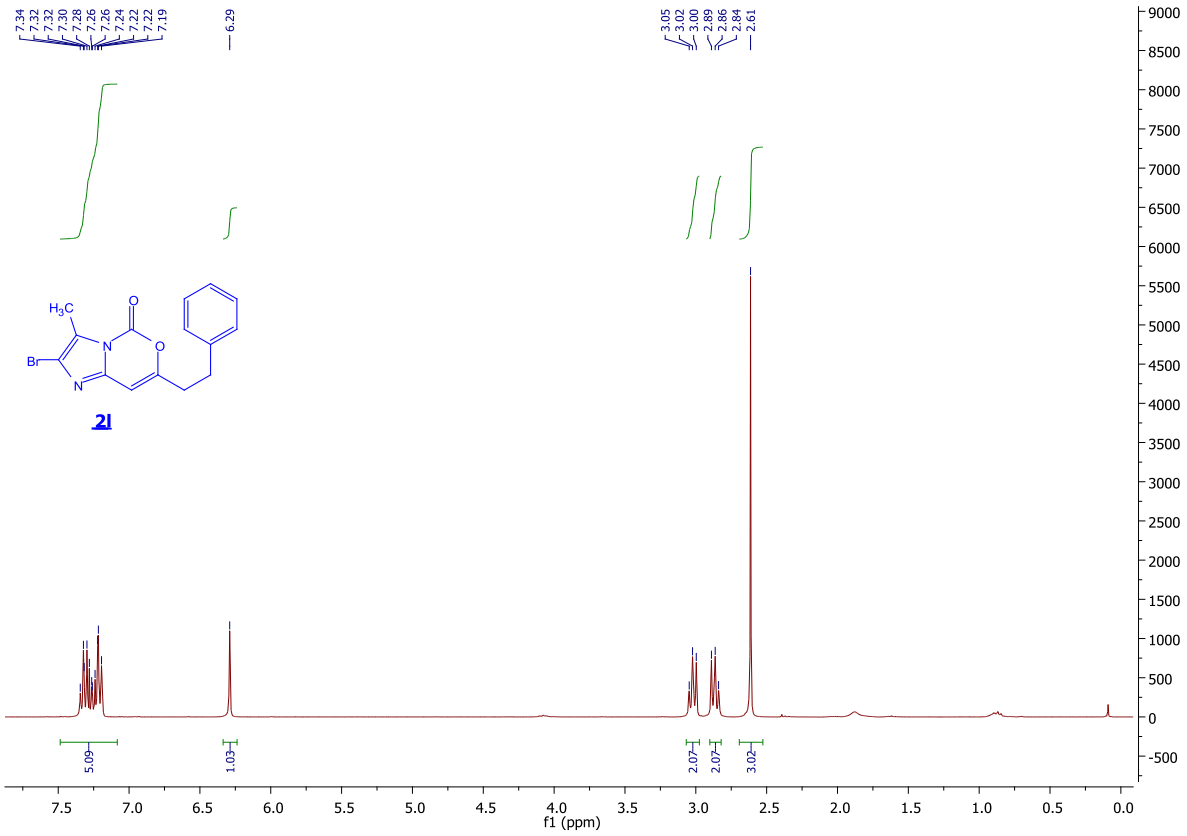

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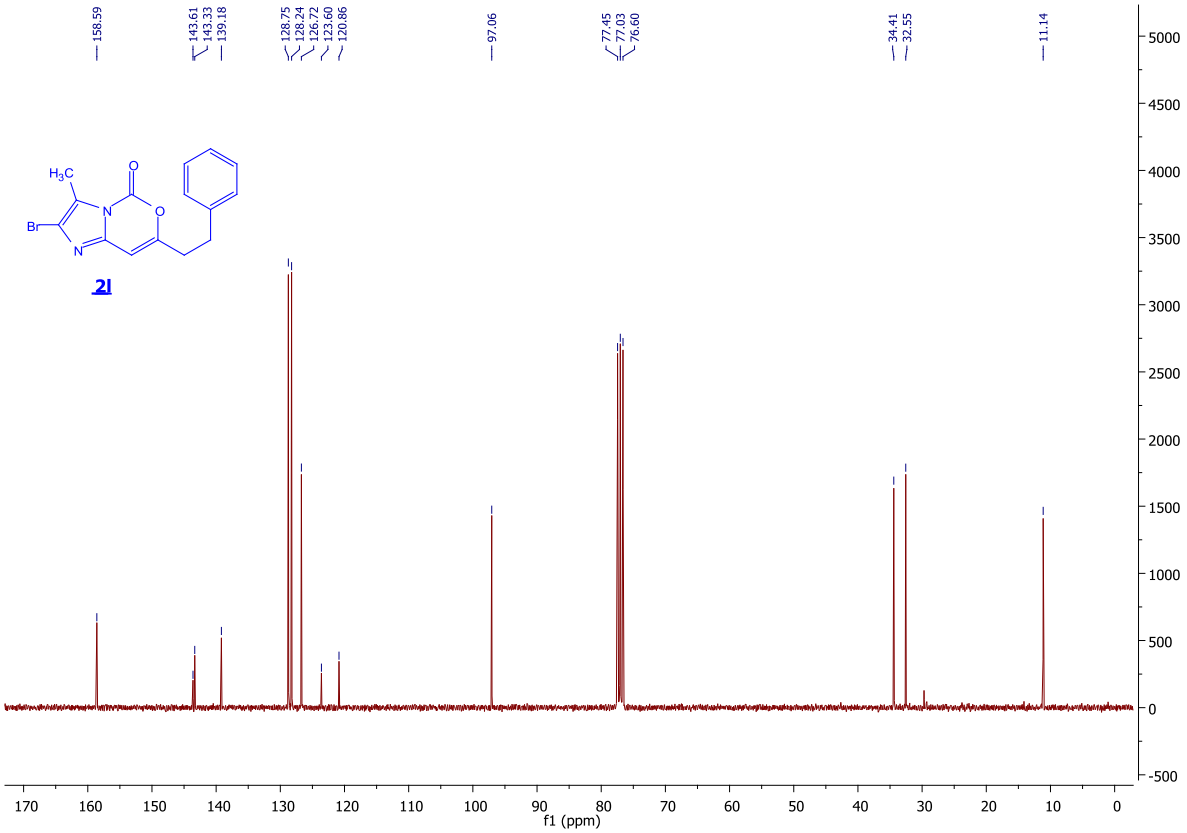
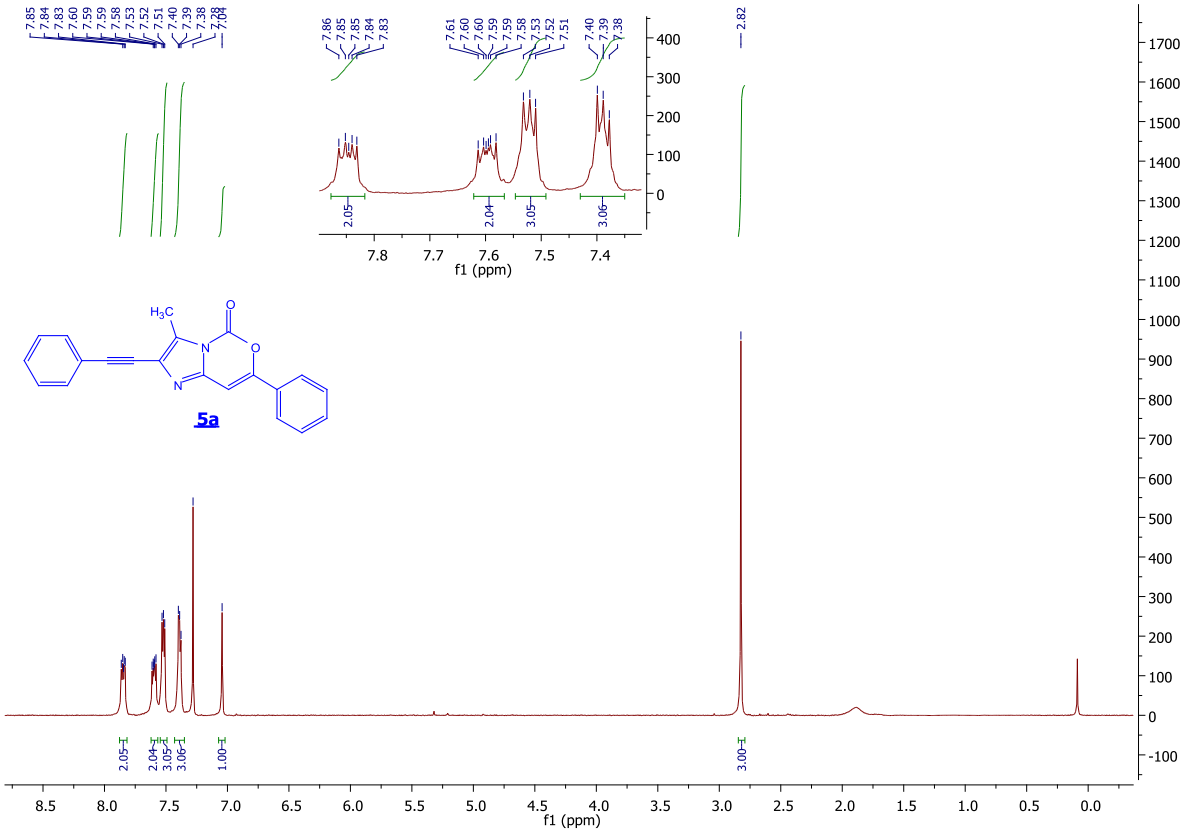


^{1}H NMR (300 MHz, $CDCl_3$) of **5a**



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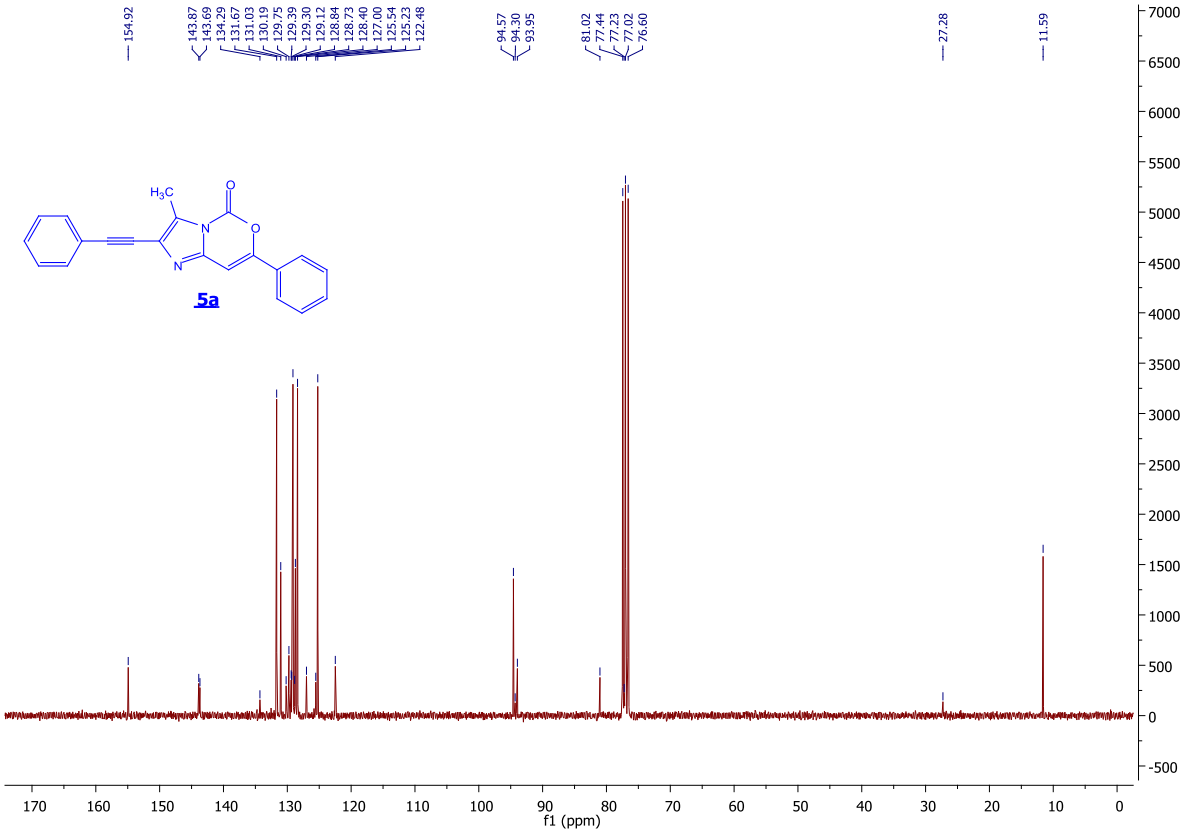
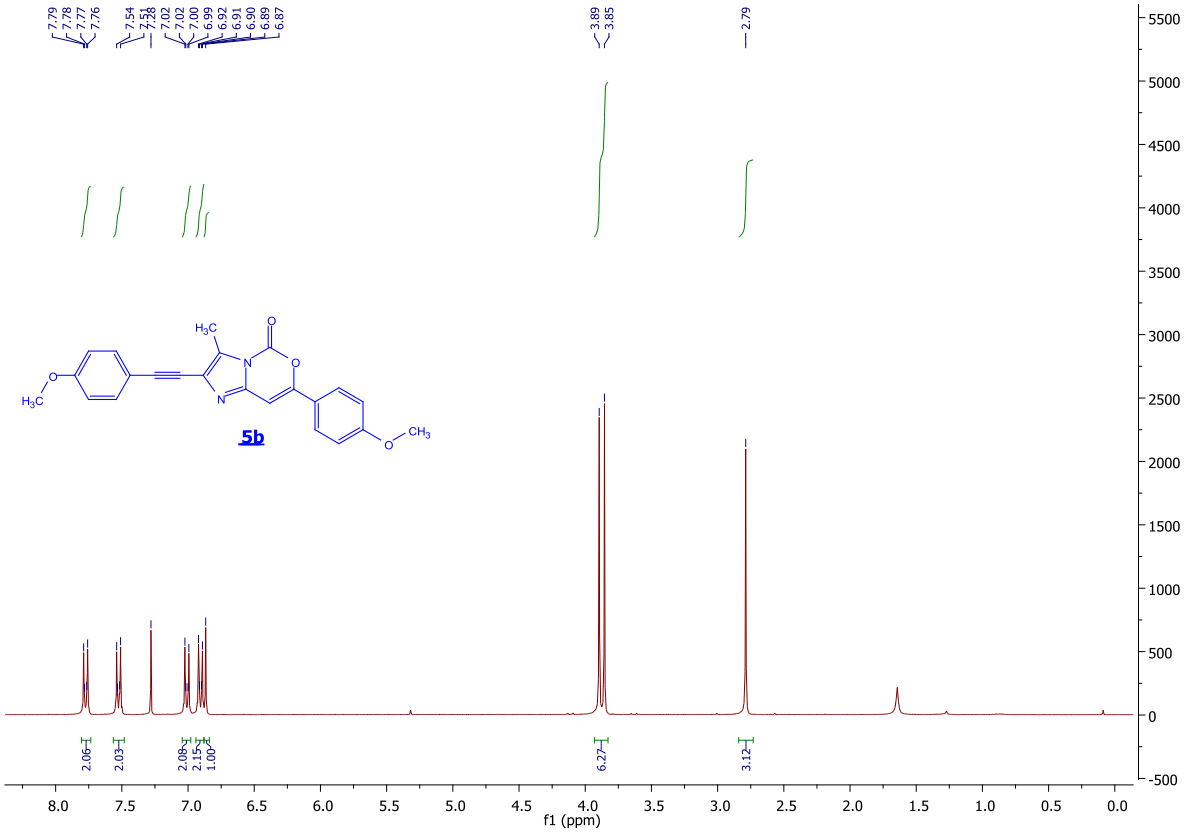
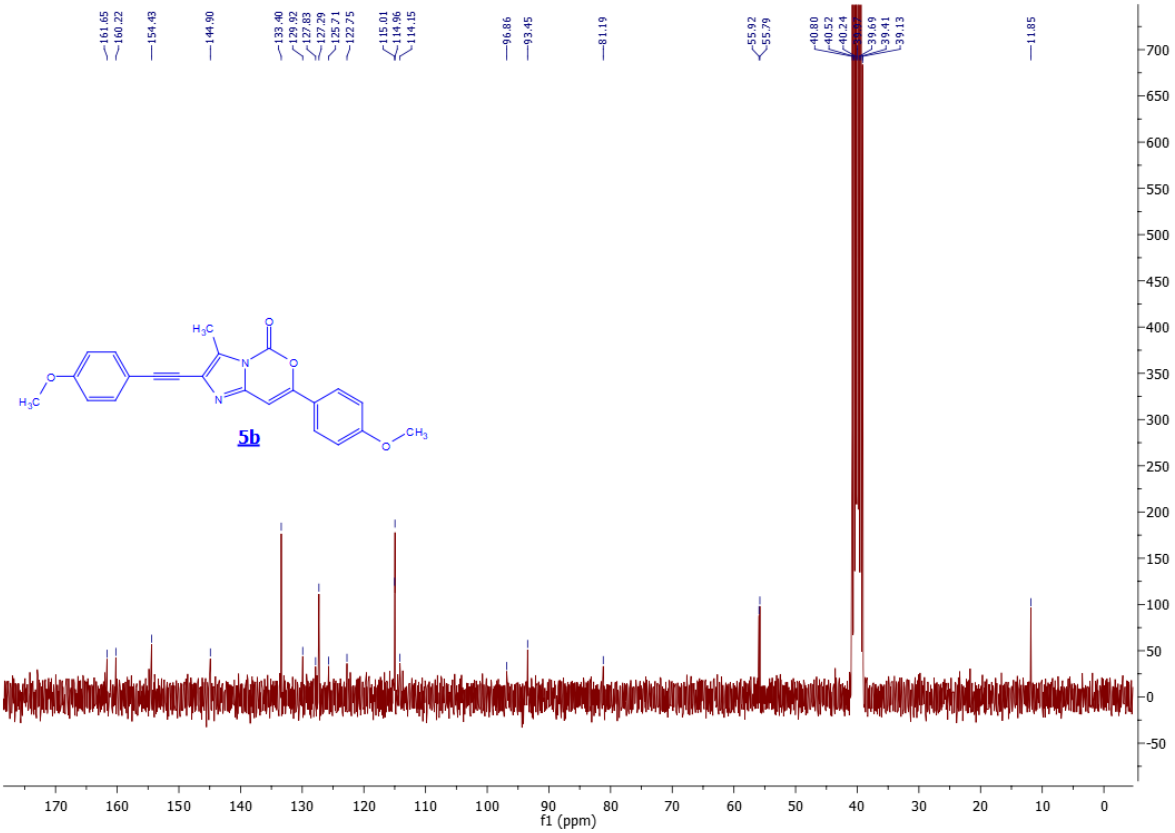


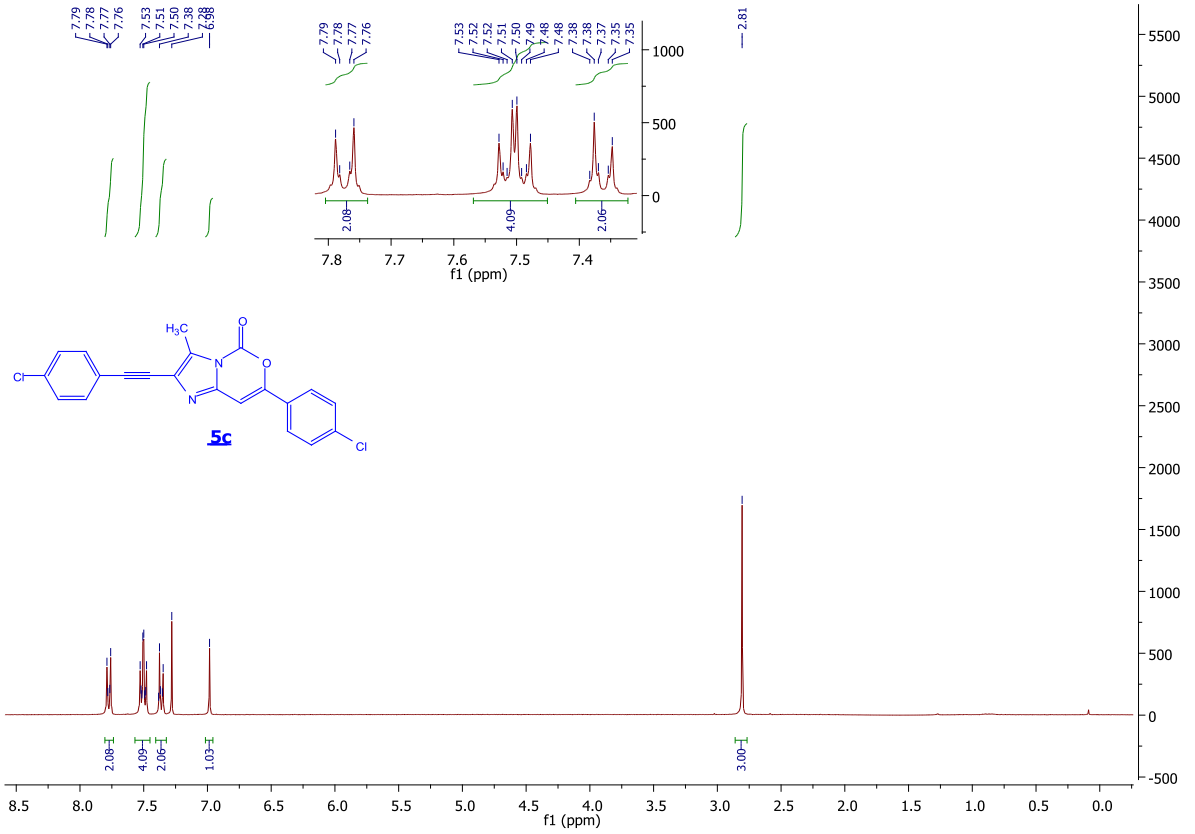
^{1}H NMR (300 MHz, $CDCl_3$) of **5b**



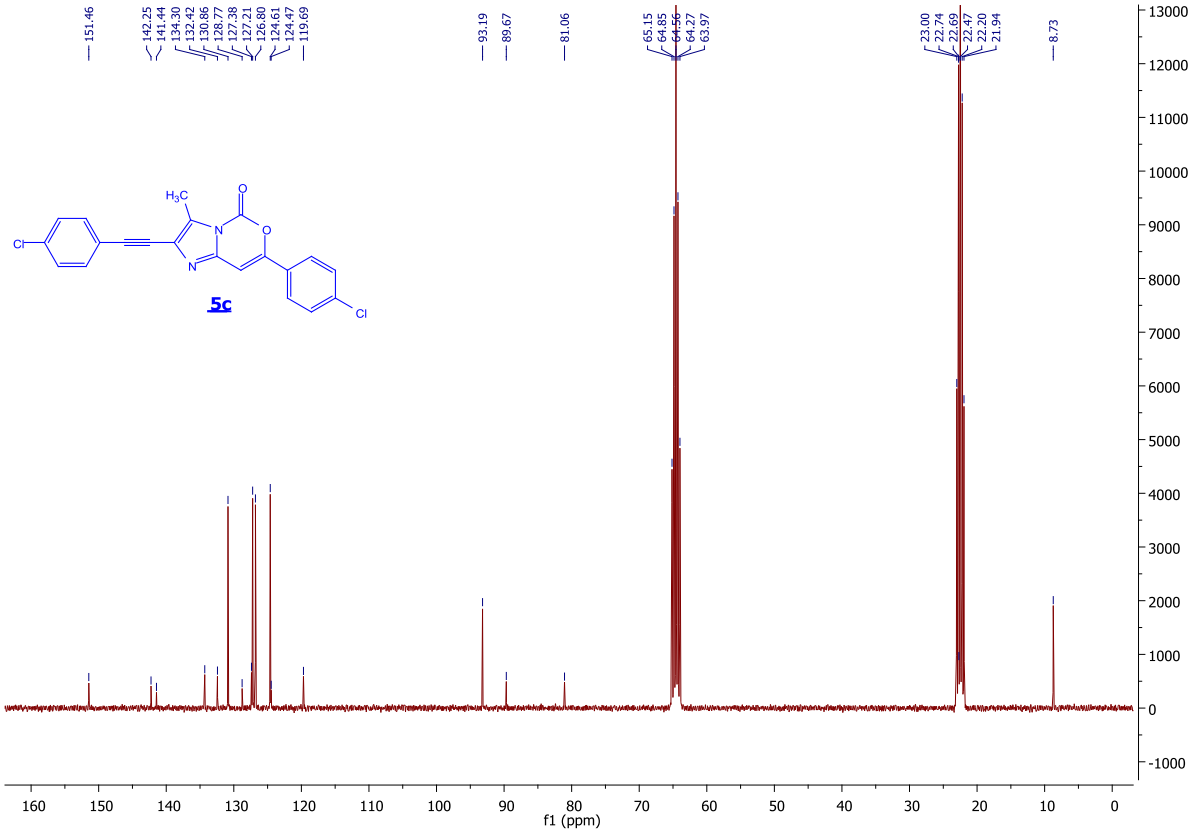
^{13}C NMR (75 MHz, DMSO-d_6) of **5b**



^{1}H NMR (300 MHz, $CDCl_3$) of **5c**



^{13}C NMR (75 MHz, THF-d_8) of **5c**



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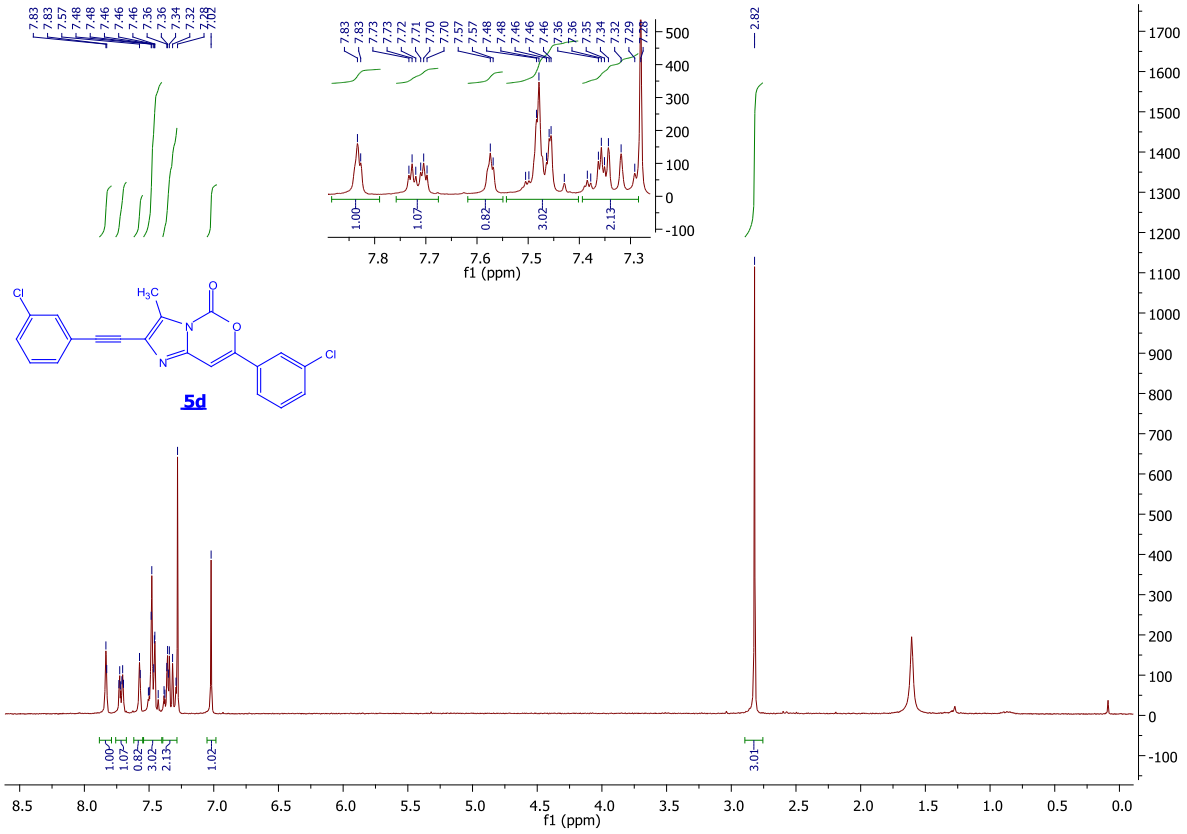
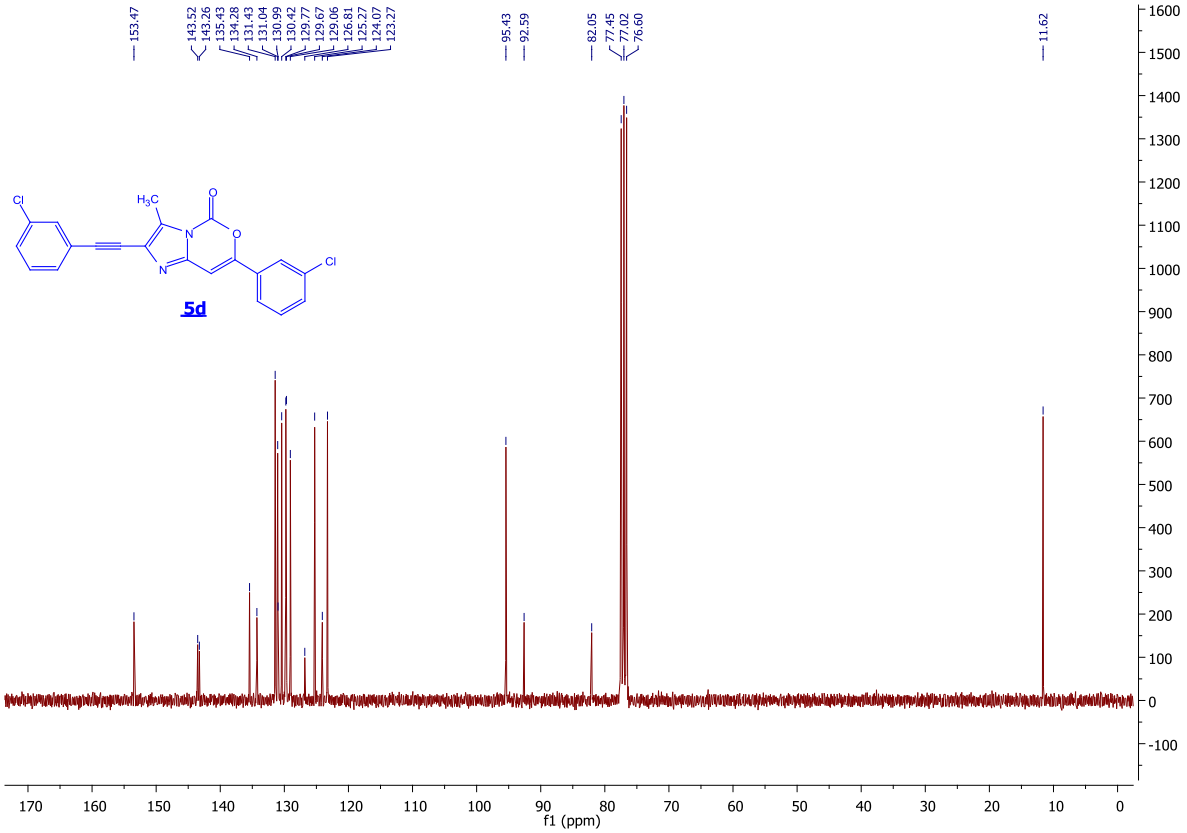


^{13}C NMR (75 MHz, $CDCl_3$) of **5d**



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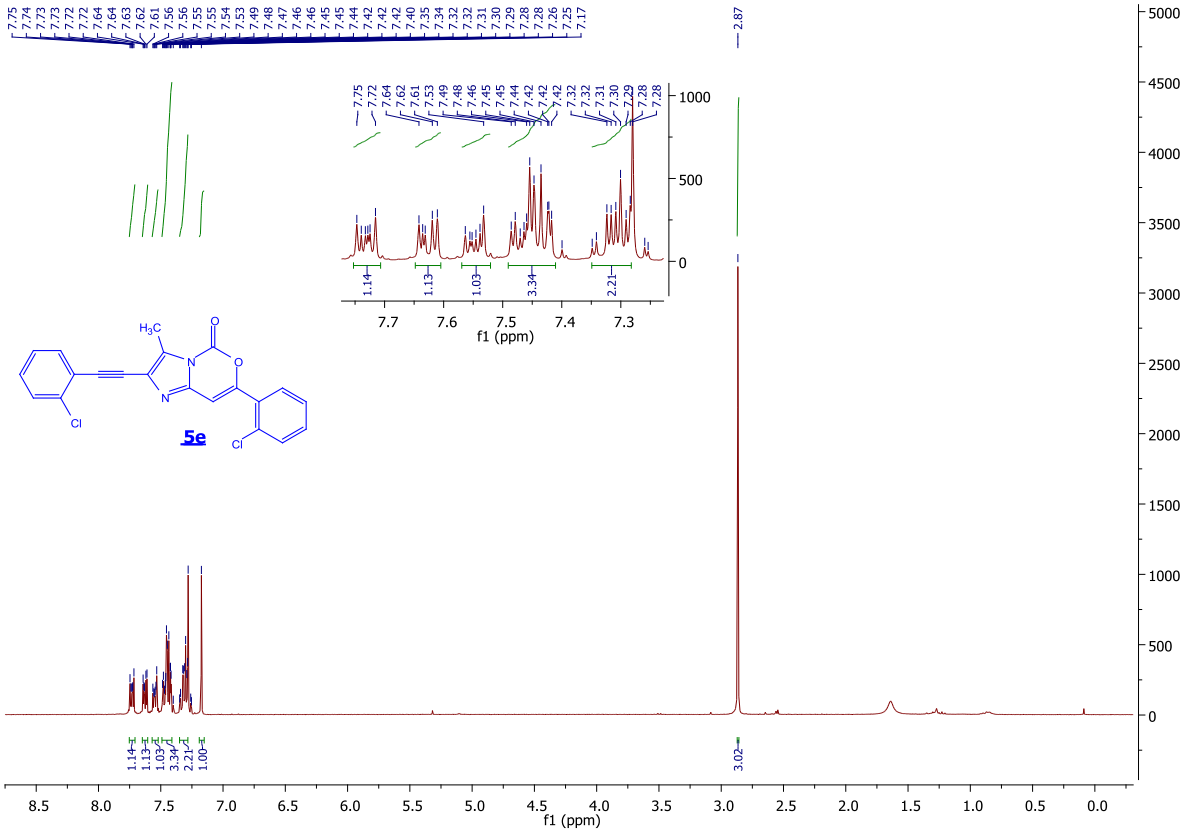
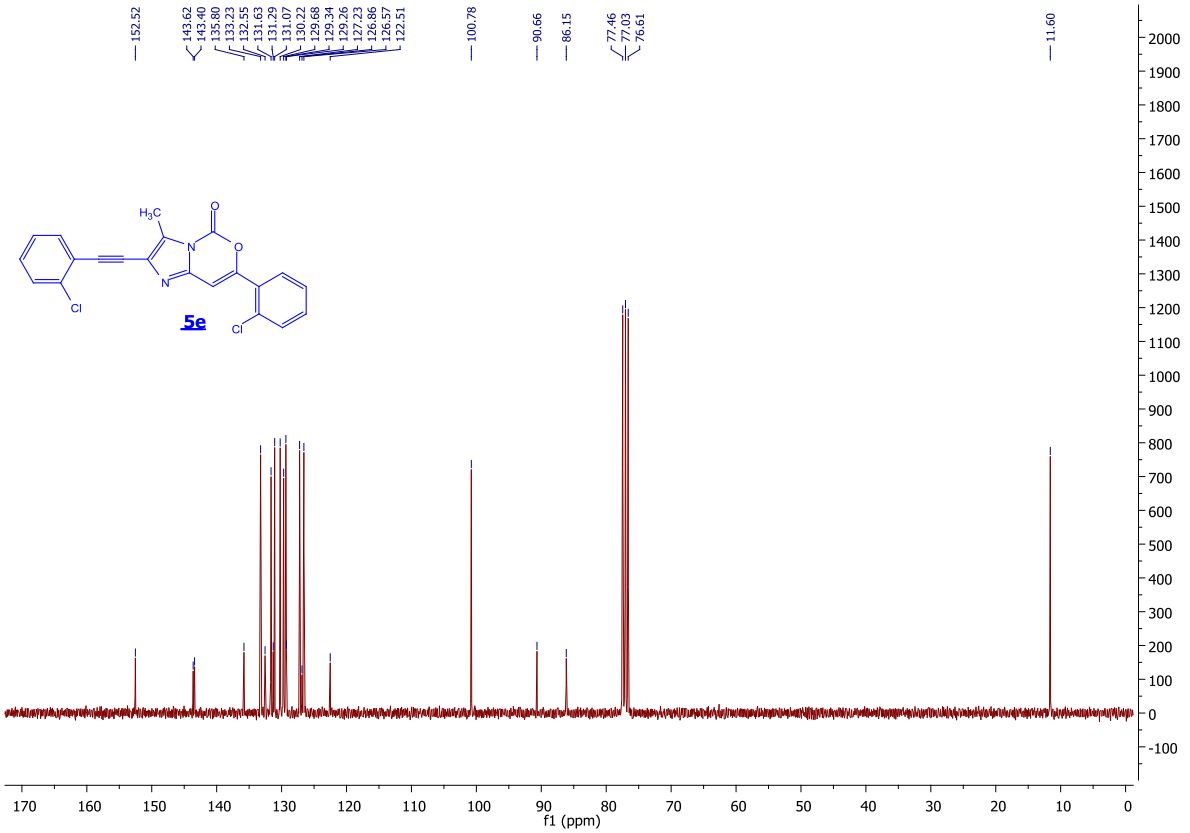
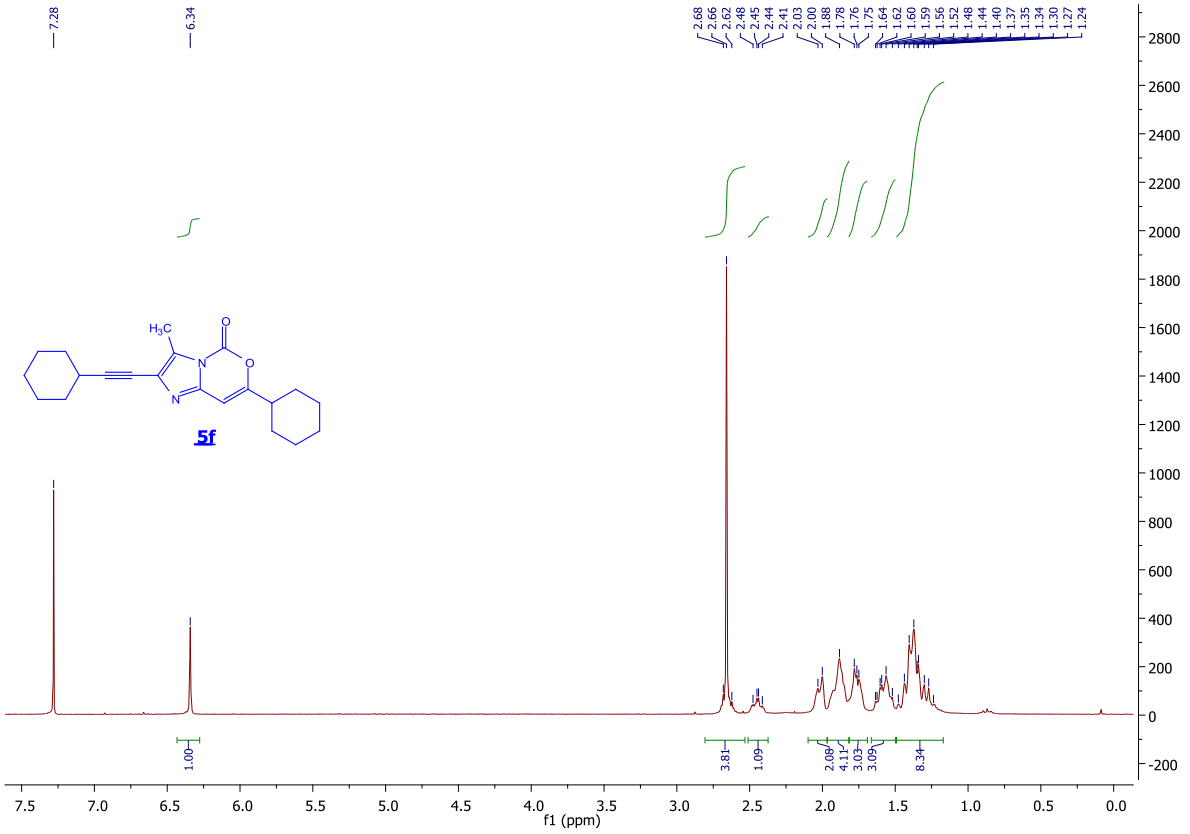


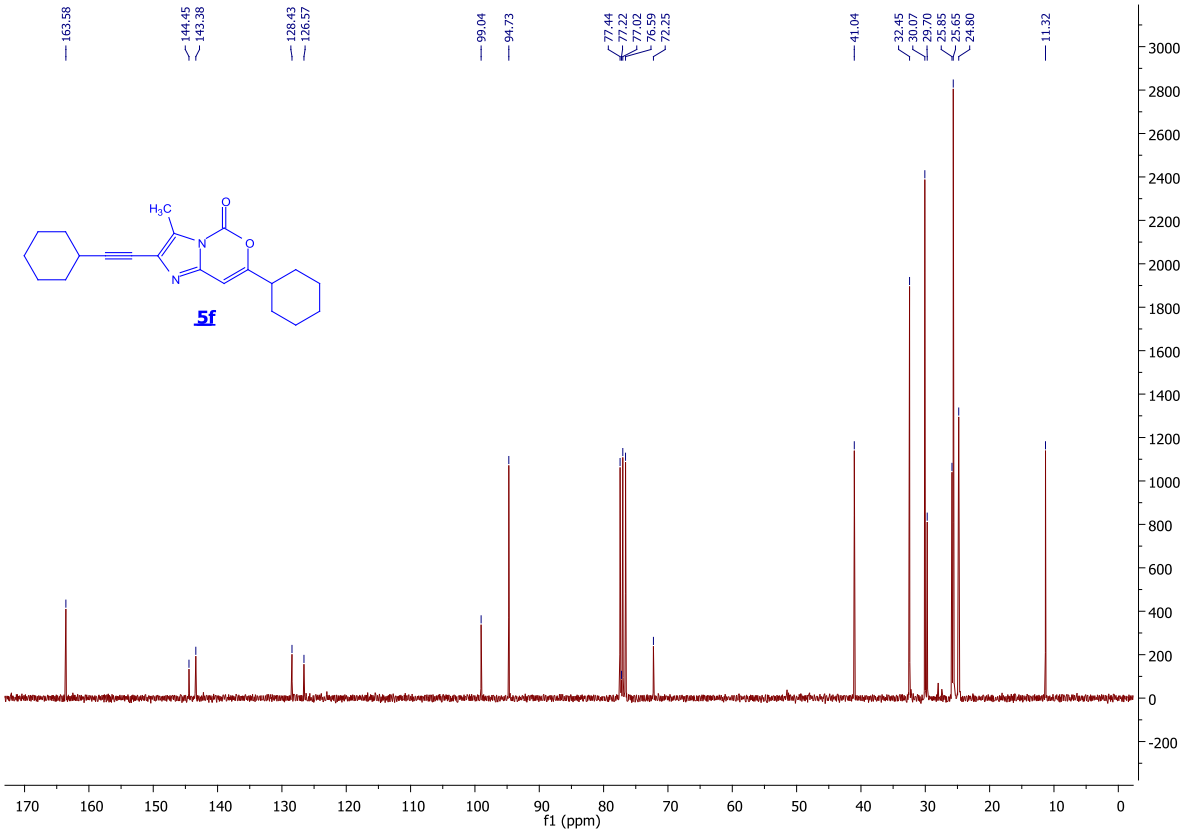
^{13}C NMR (75 MHz, $CDCl_3$) of **5e**



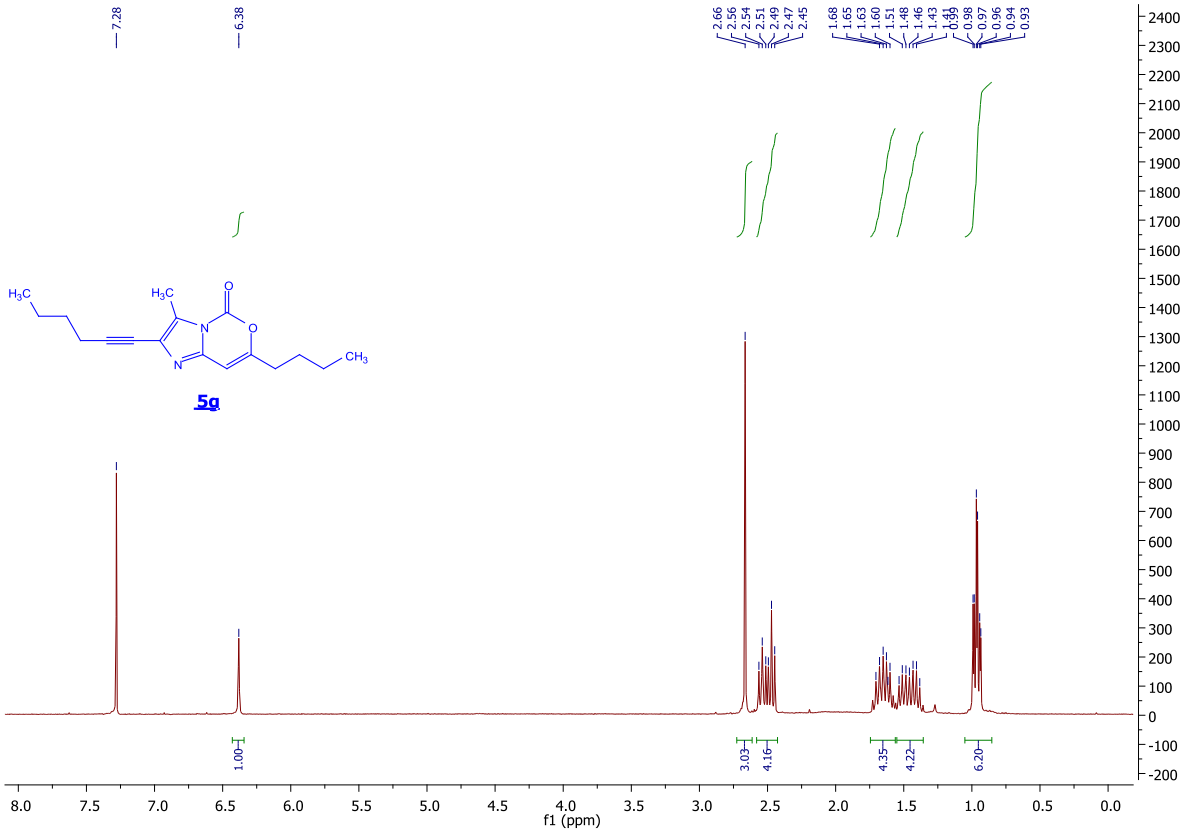
^{1}H NMR (300 MHz, $CDCl_3$) of **5f**



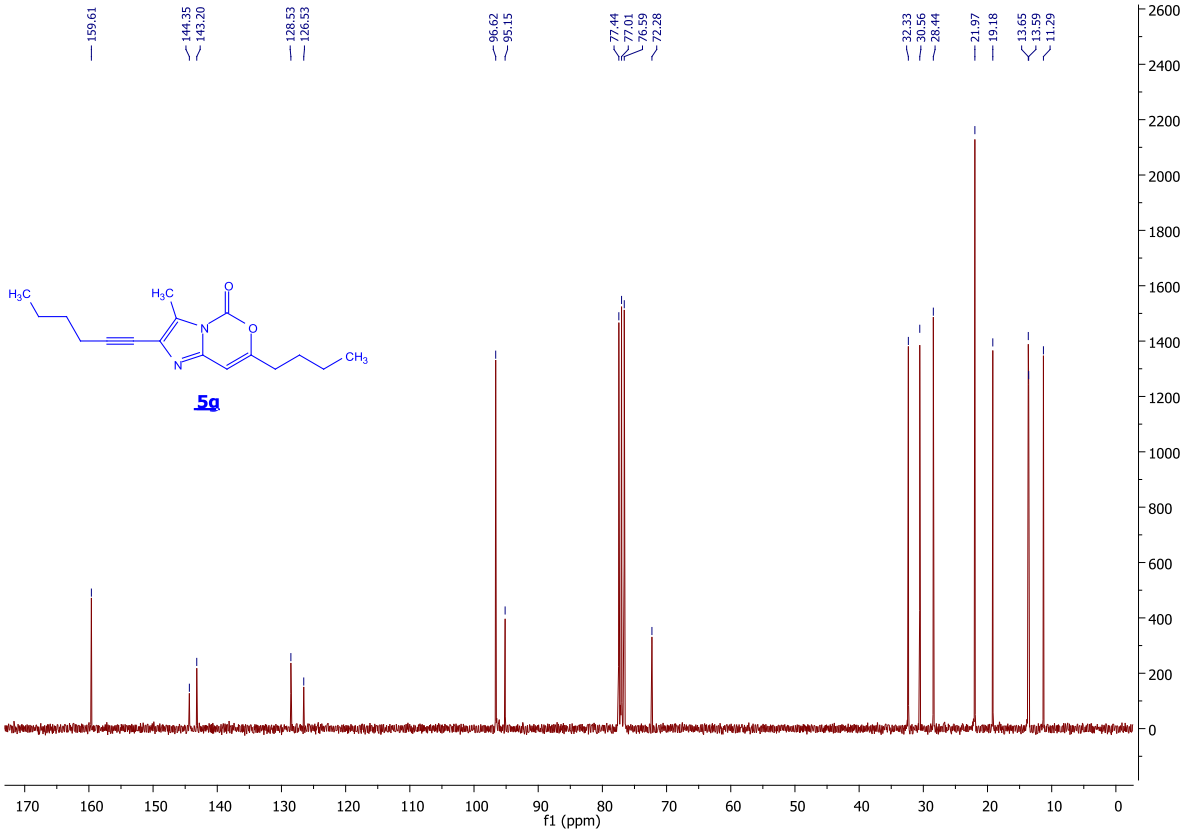
^{13}C NMR (75 MHz, $CDCl_3$) of **5f**



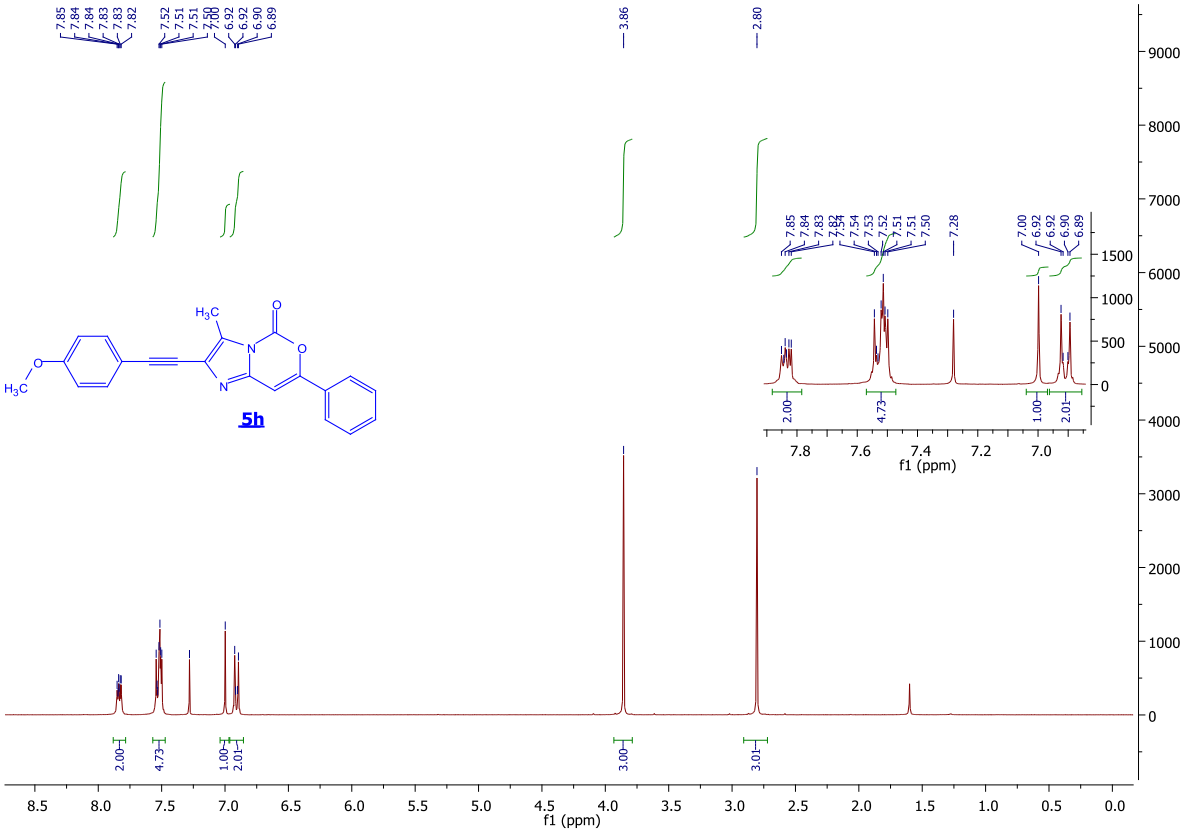
^{1}H NMR (300 MHz, $CDCl_3$) of **5g**



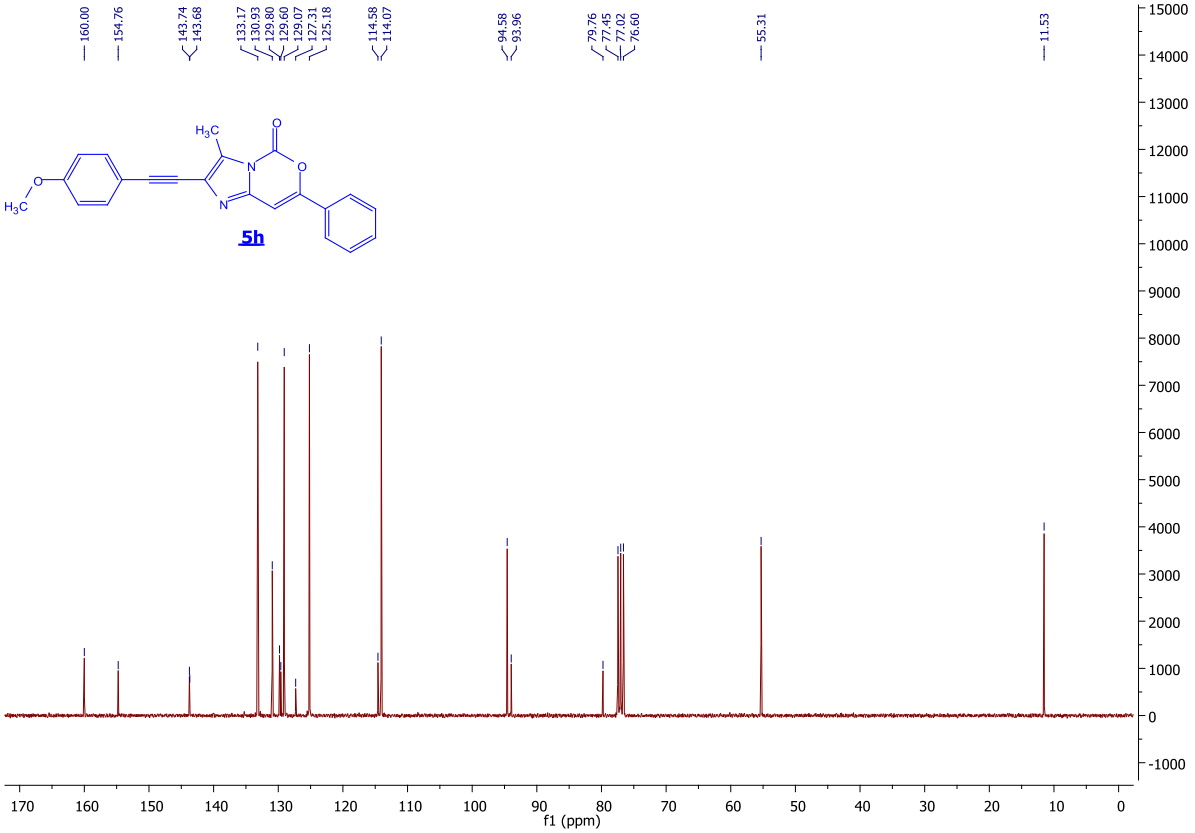
^{13}C NMR (75 MHz, $CDCl_3$) of **5g**



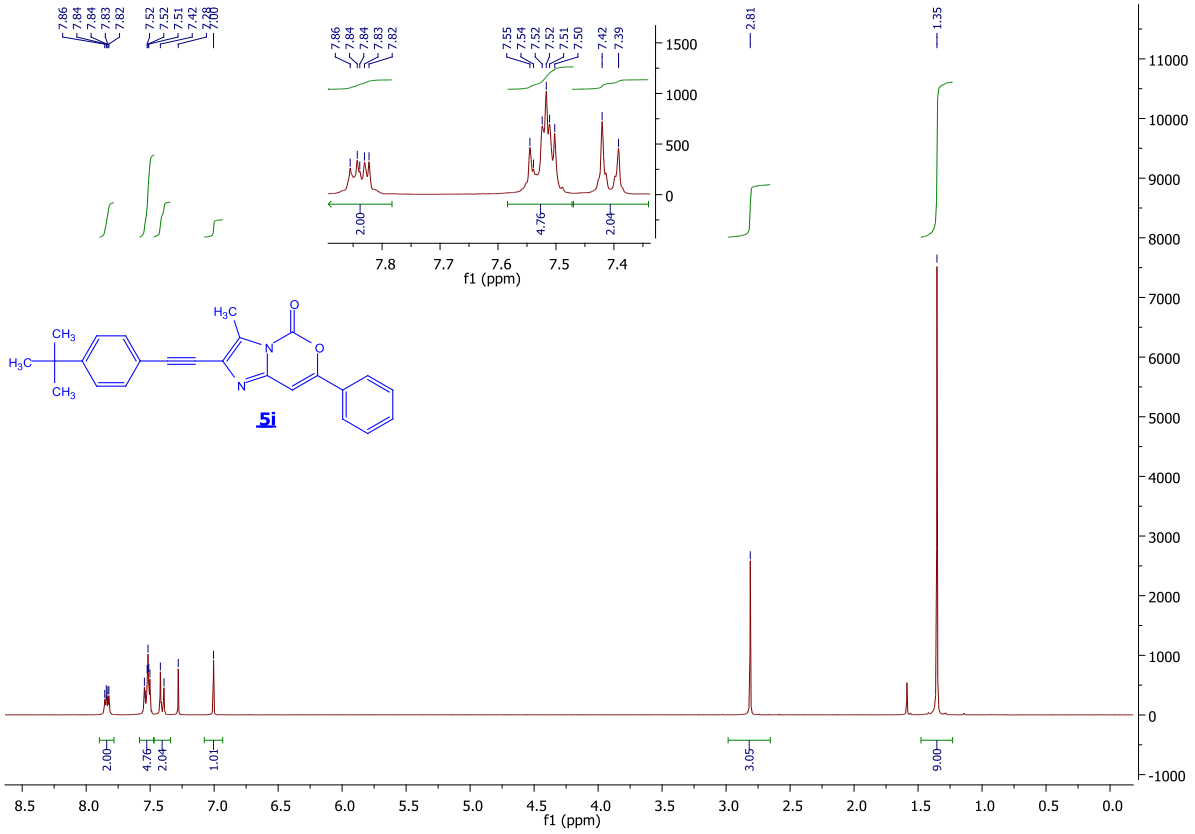
^{1}H NMR (300 MHz, $CDCl_3$) of **5h**



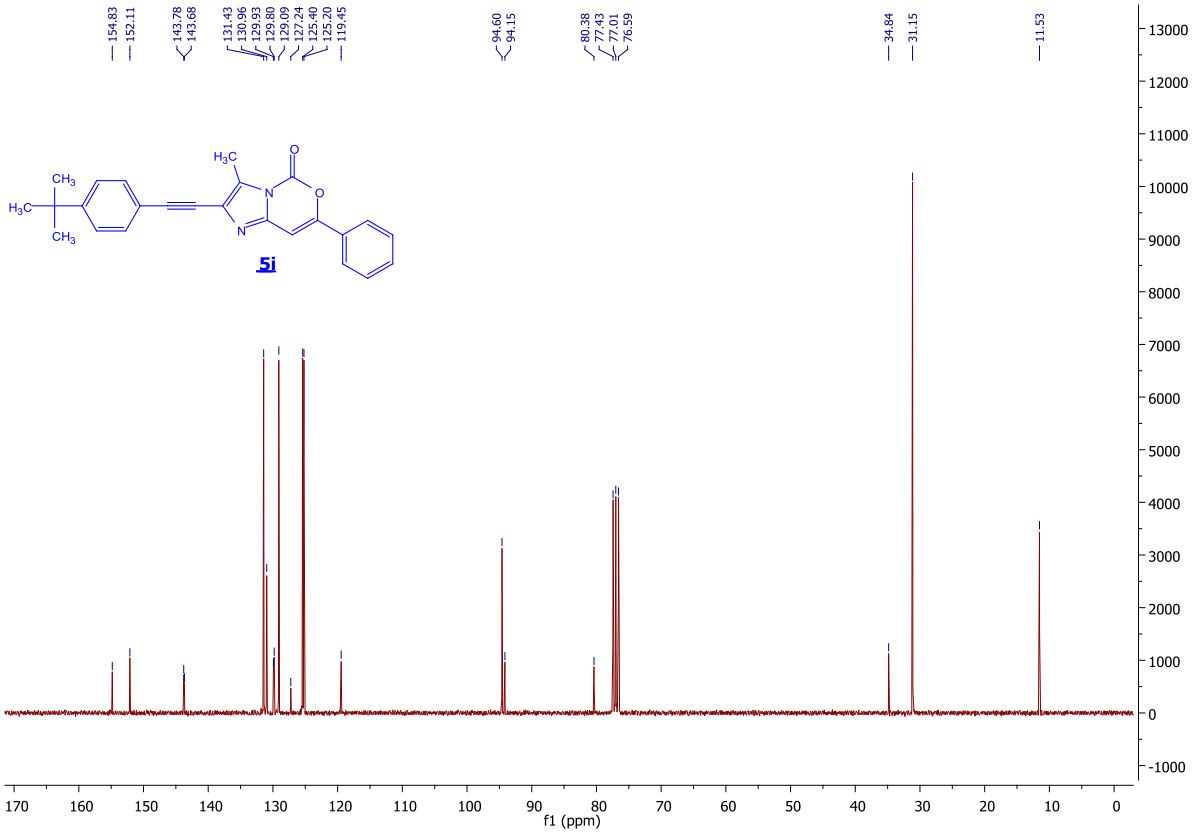
^{13}C NMR (75 MHz, $CDCl_3$) of **5h**



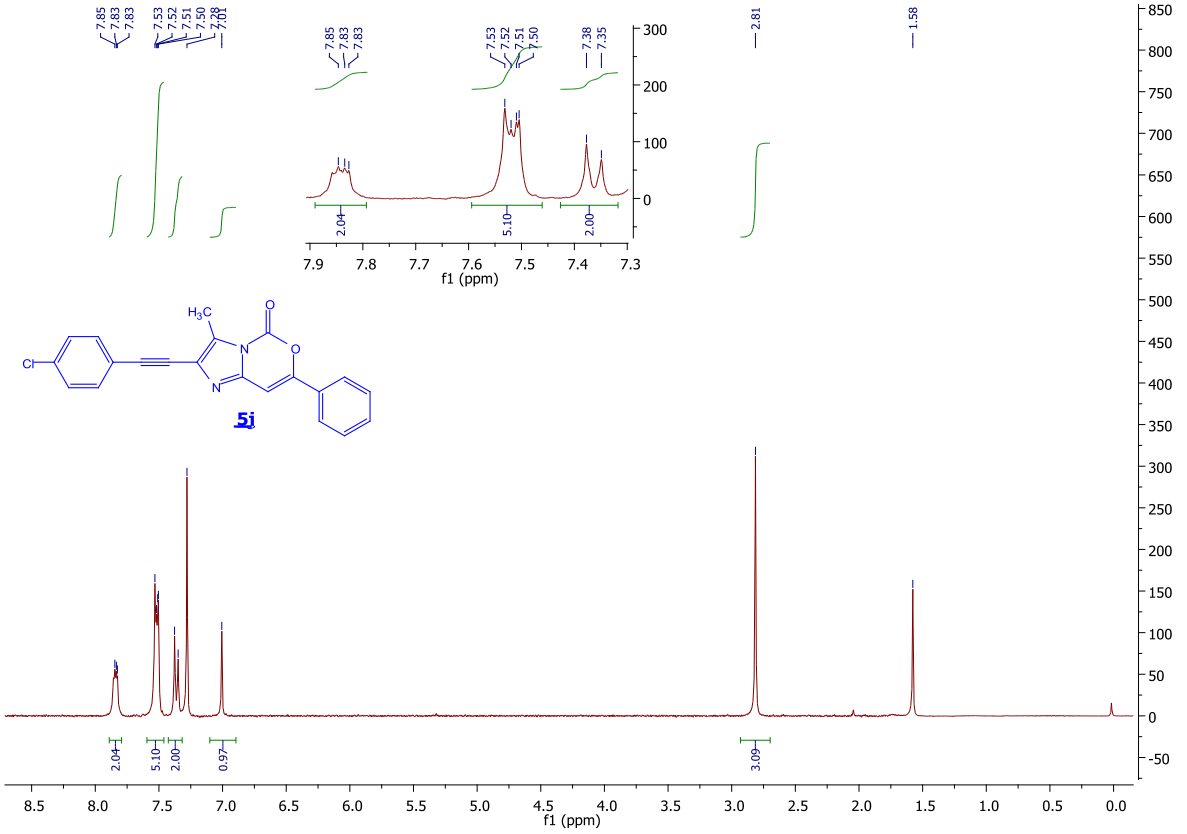
^{1}H NMR (300 MHz, $CDCl_3$) of **5i**



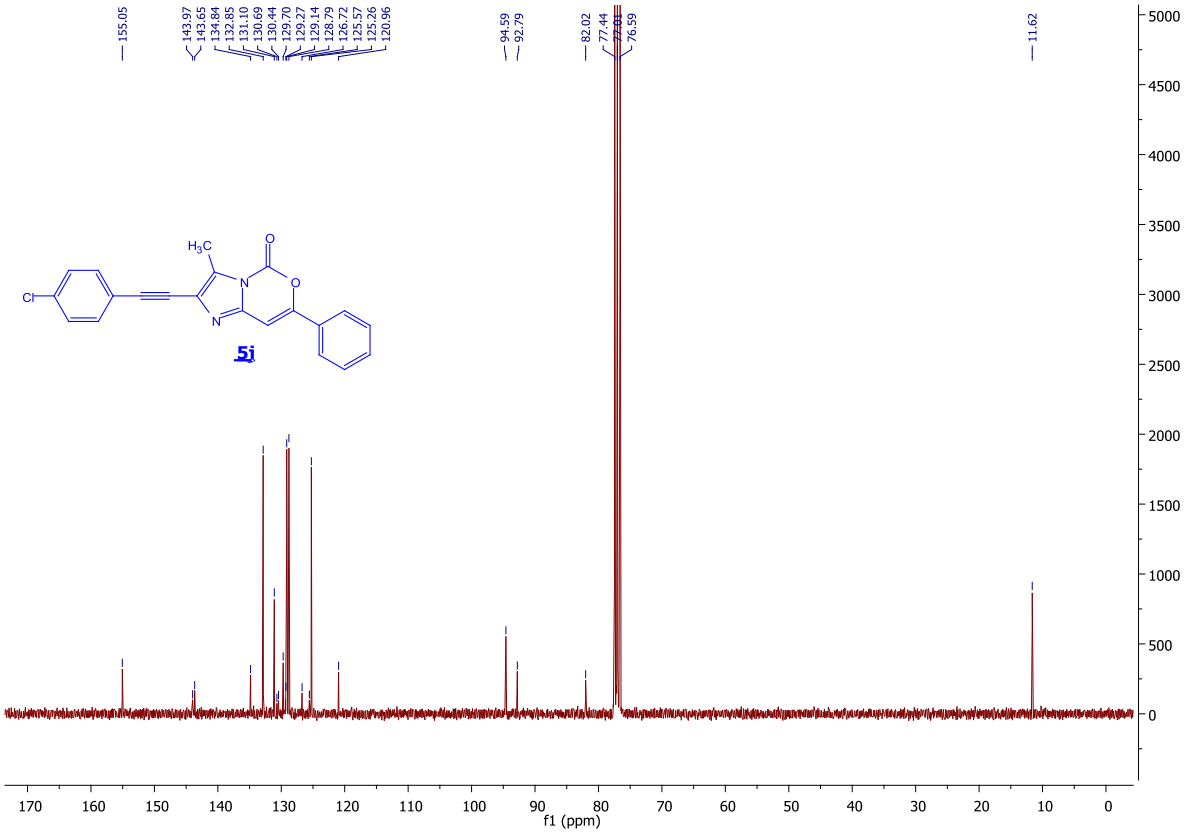
^{13}C NMR (75 MHz, $CDCl_3$) of **5i**



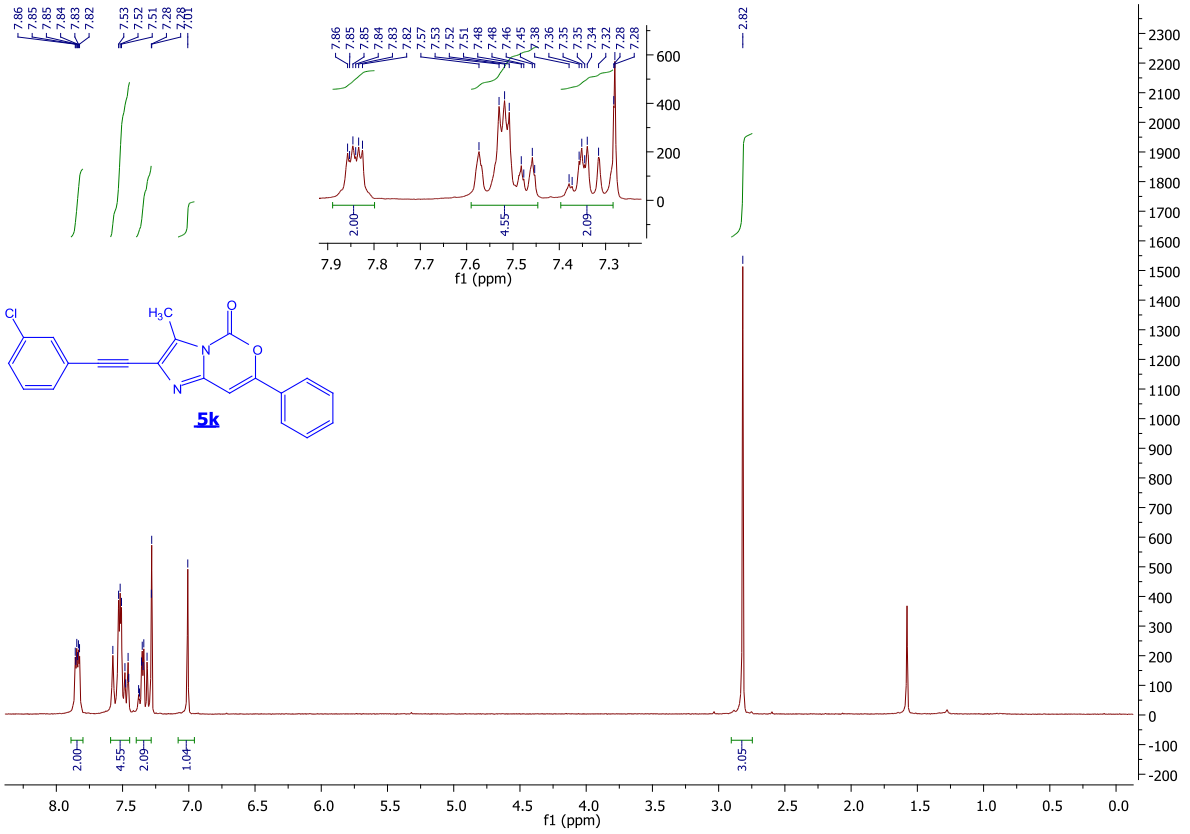
^{1}H NMR (300 MHz, $CDCl_3$) of **5j**



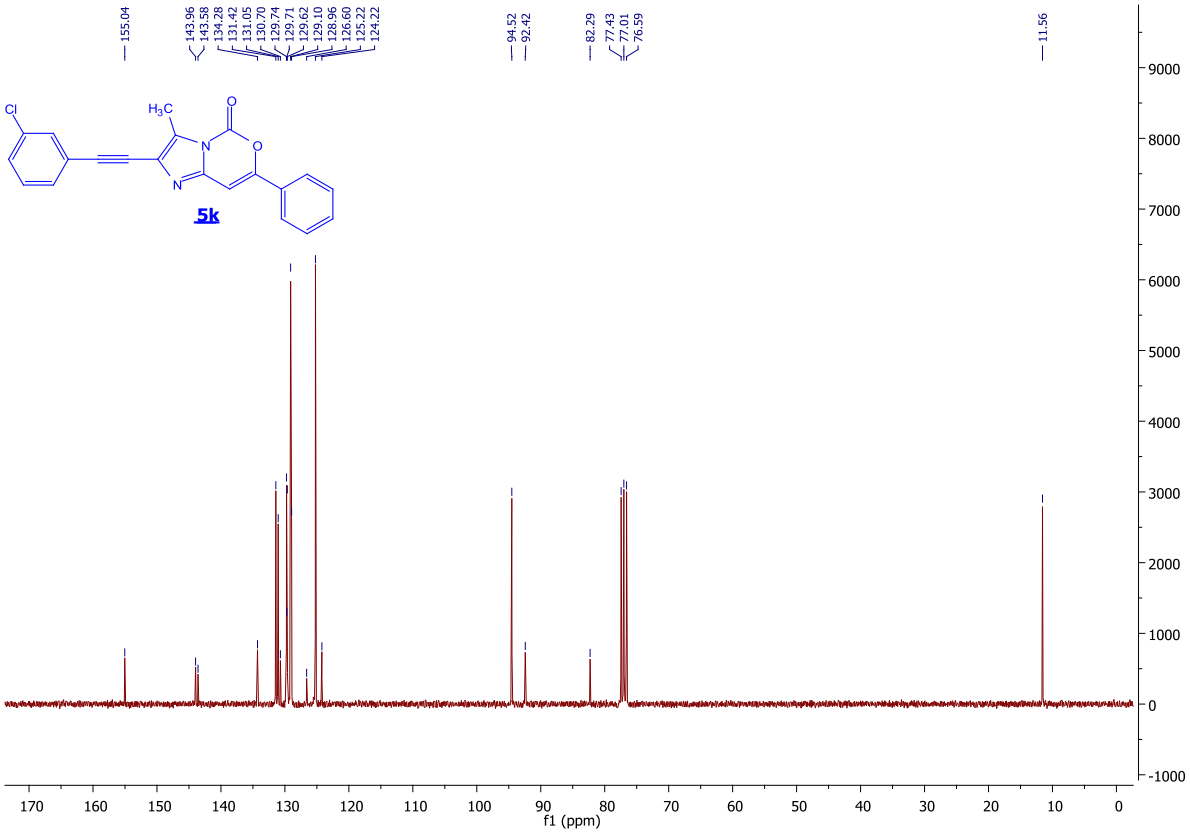
^{13}C NMR (75 MHz, $CDCl_3$) of **5j**



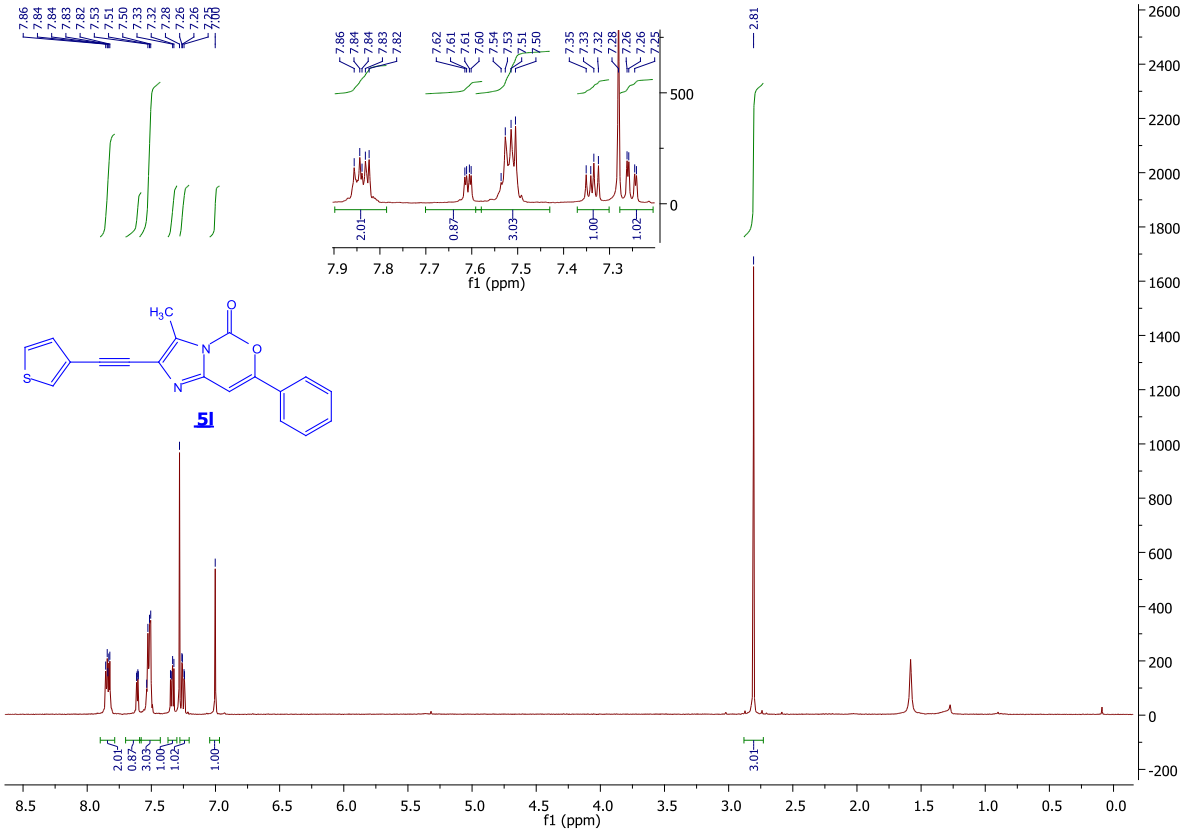
^{1}H NMR (300 MHz, $CDCl_3$) of **5k**



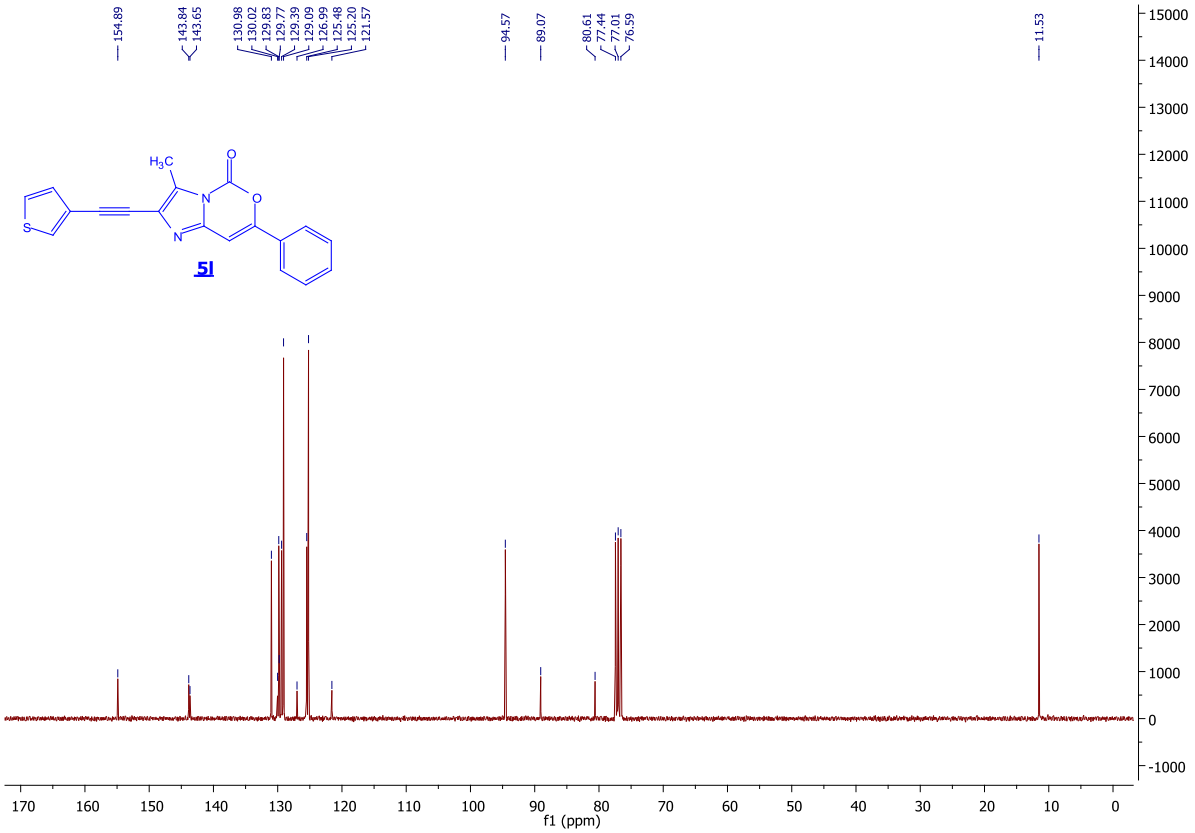
^{13}C NMR (75 MHz, $CDCl_3$) of **5k**



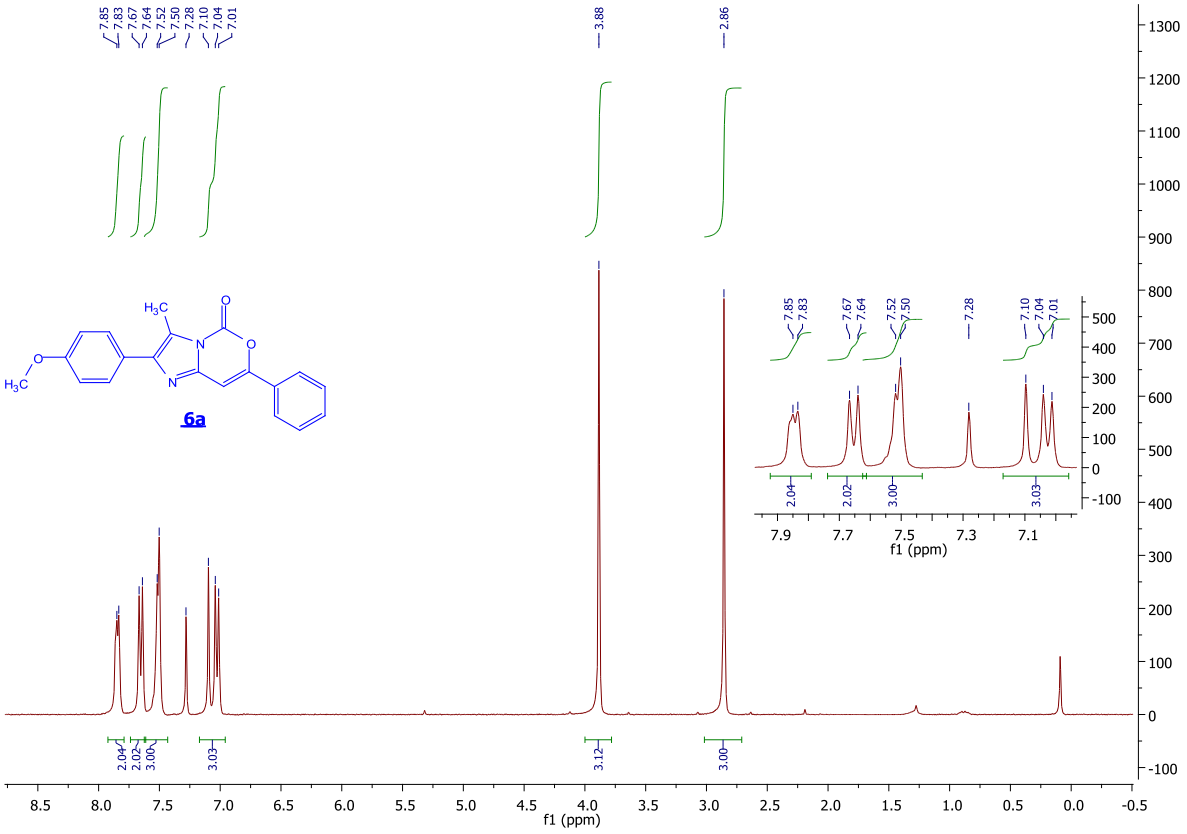
^{1}H NMR (300 MHz, $CDCl_3$) of **5l**



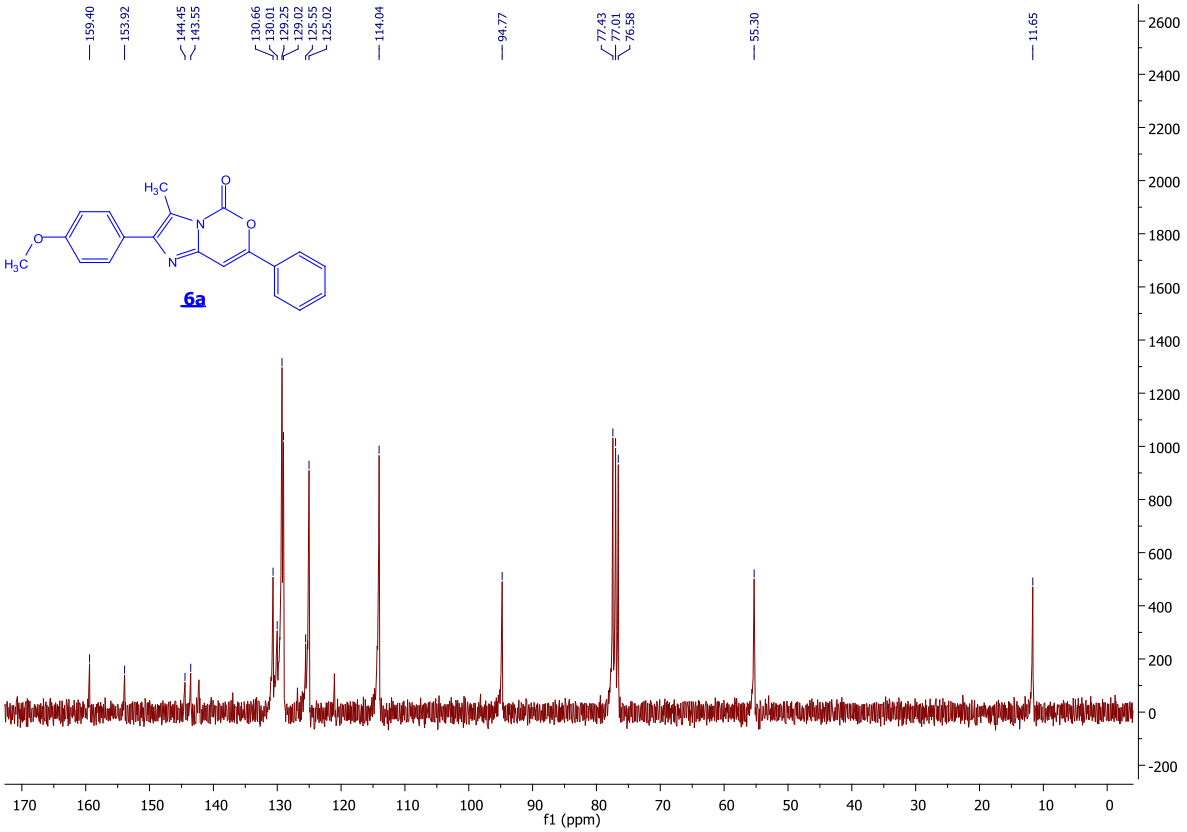
^{13}C NMR (75 MHz, $CDCl_3$) of **5l**



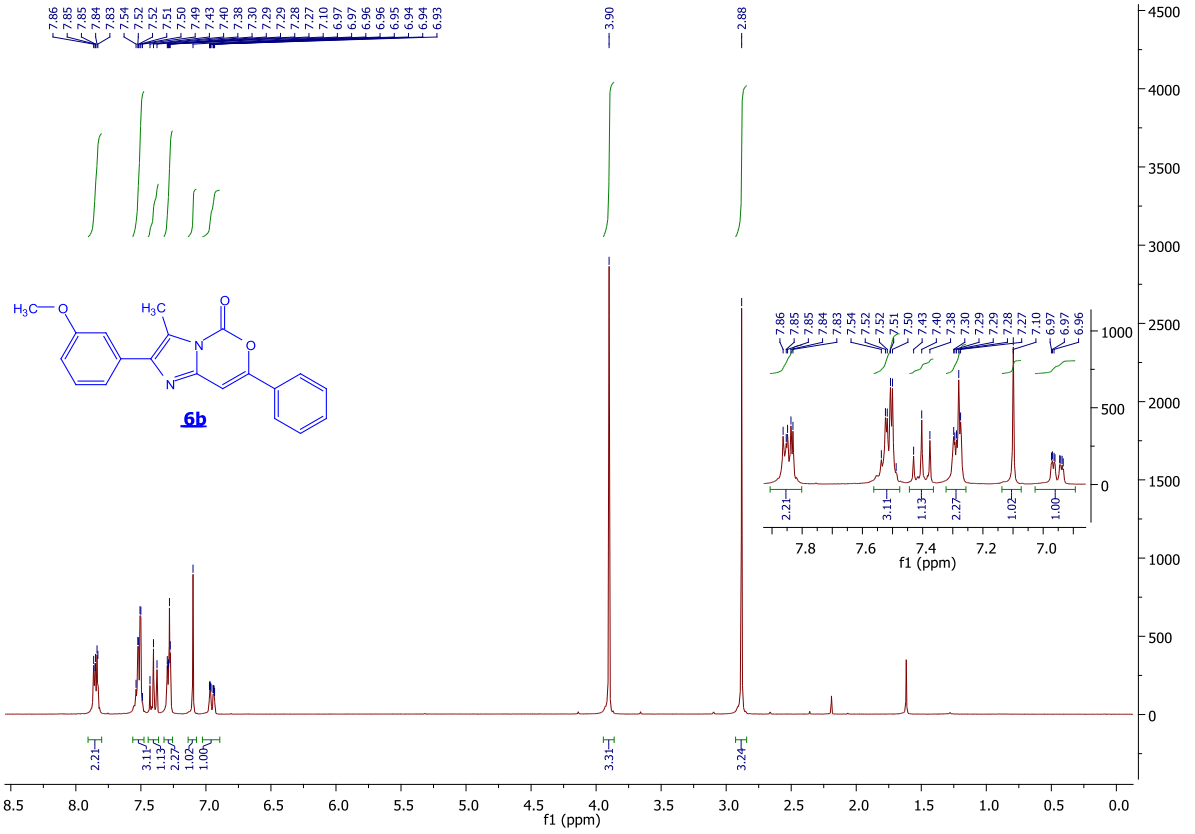
^{1}H NMR (300 MHz, $CDCl_3$) of **6a**



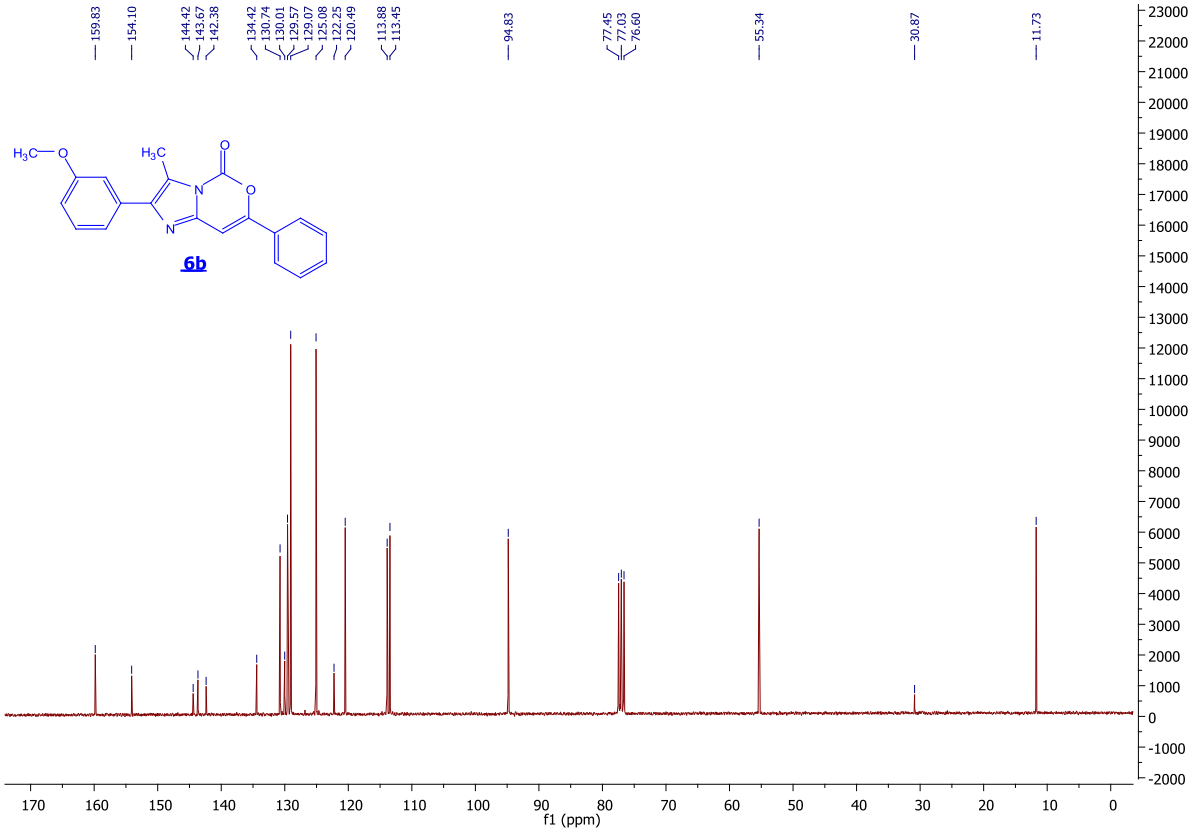
^{13}C NMR (75 MHz, $CDCl_3$) of **6a**



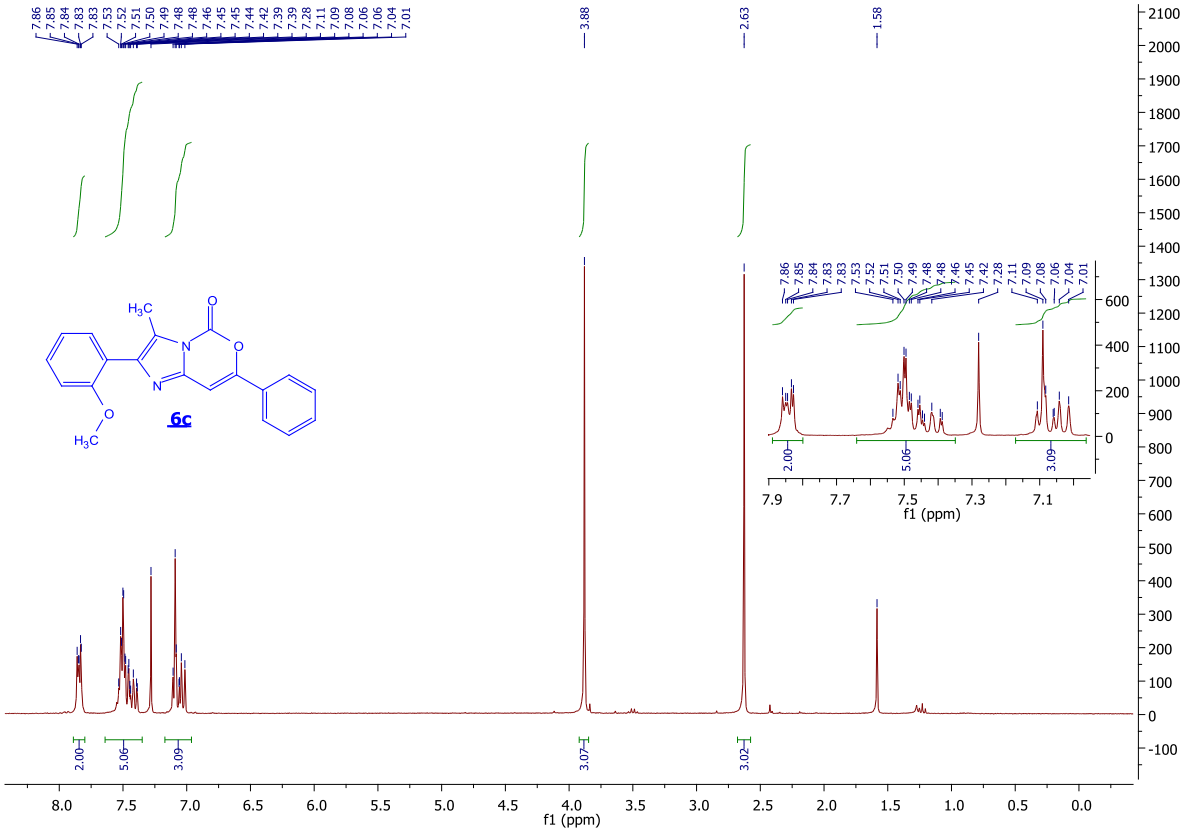
^{1}H NMR (300 MHz, $CDCl_3$) of **6b**



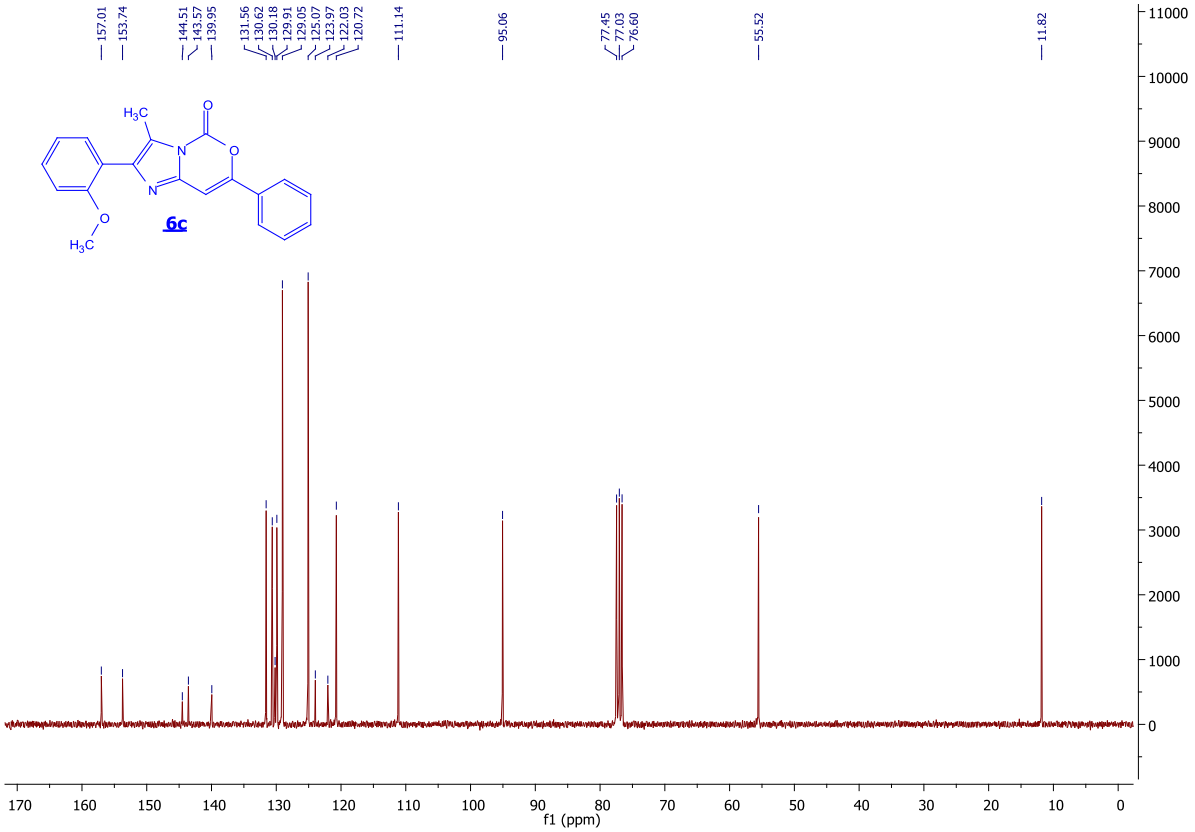
^{13}C NMR (75 MHz, $CDCl_3$) of **6b**



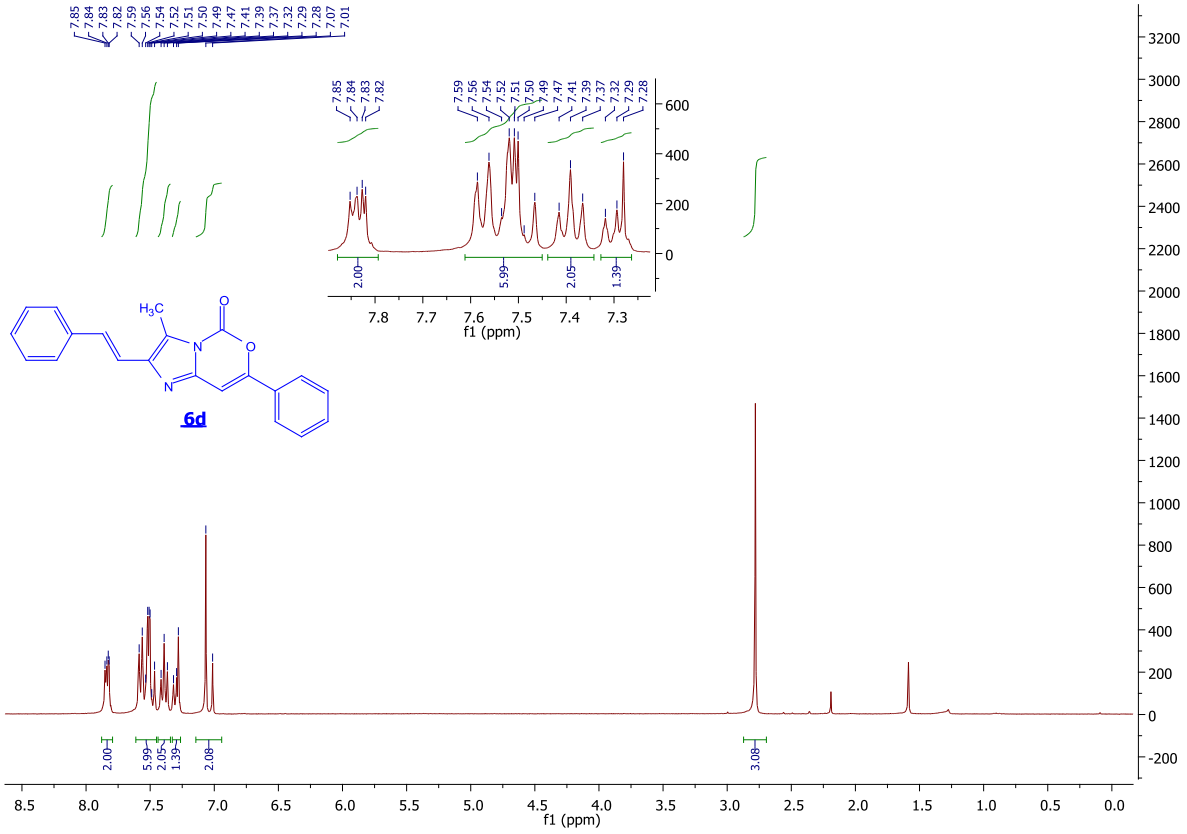
^{1}H NMR (300 MHz, $CDCl_3$) of **6c**



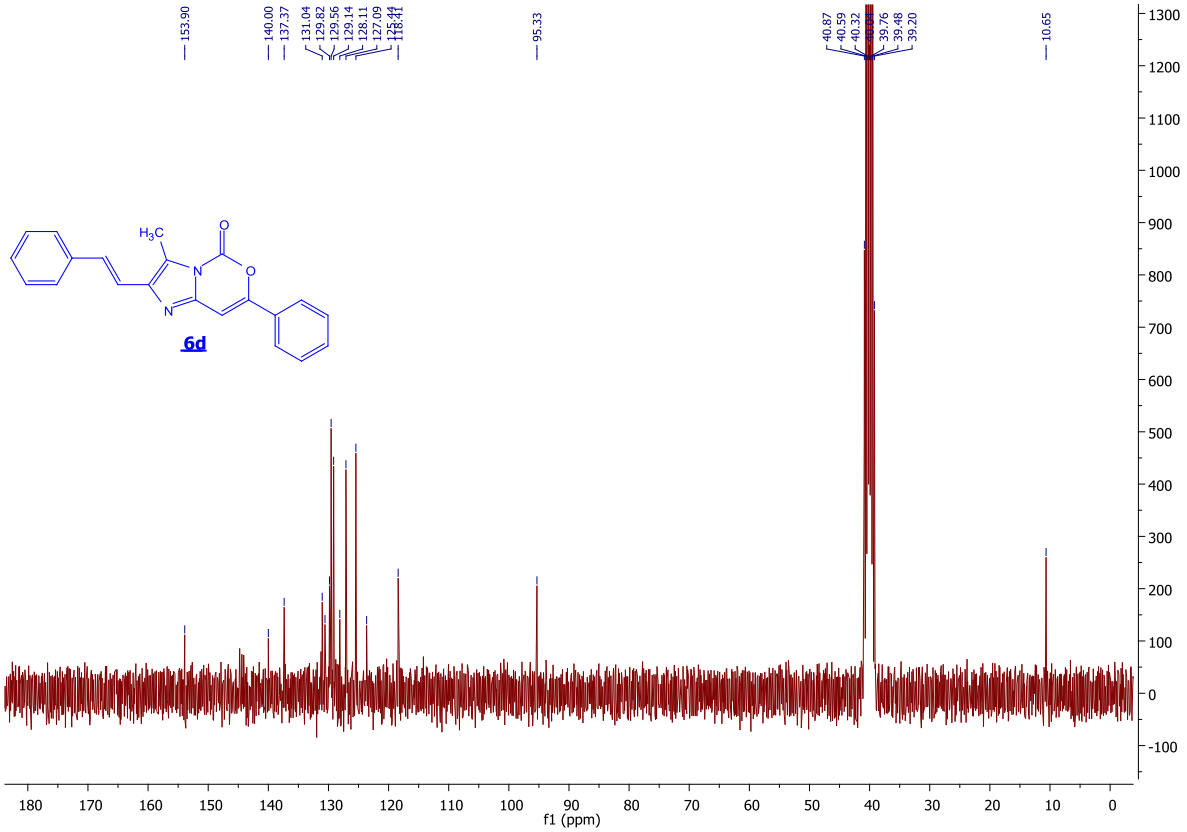
^{13}C NMR (75 MHz, $CDCl_3$) of **6c**



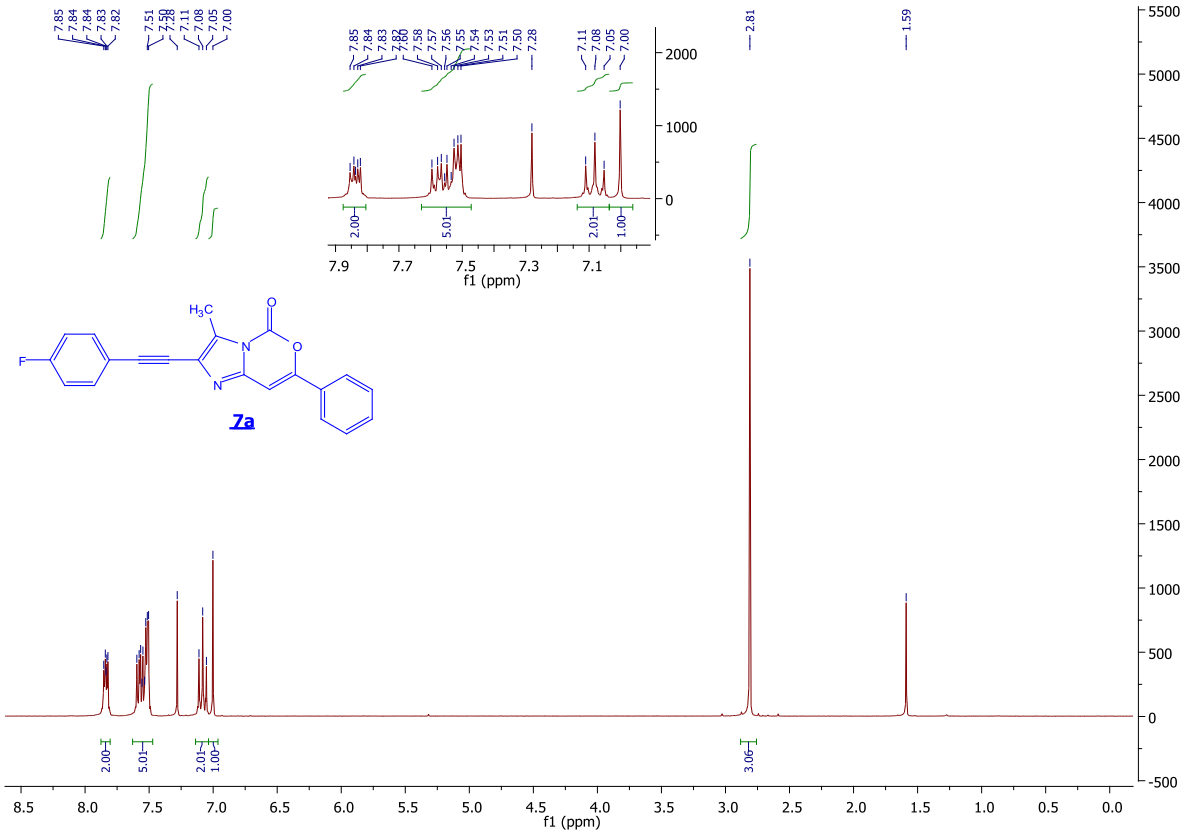
^{1}H NMR (300 MHz, $CDCl_3$) of **6d**



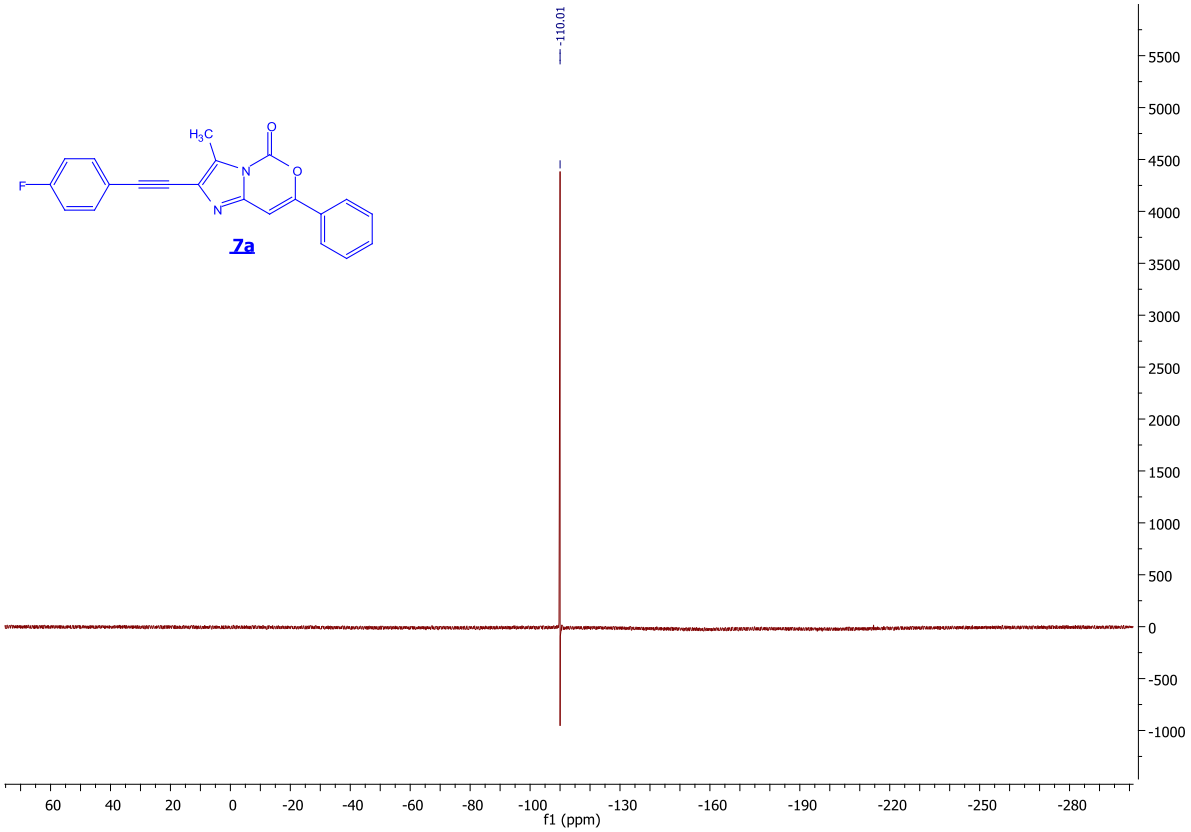
^{13}C NMR (75 MHz, DMSO-d_6) of **6d**



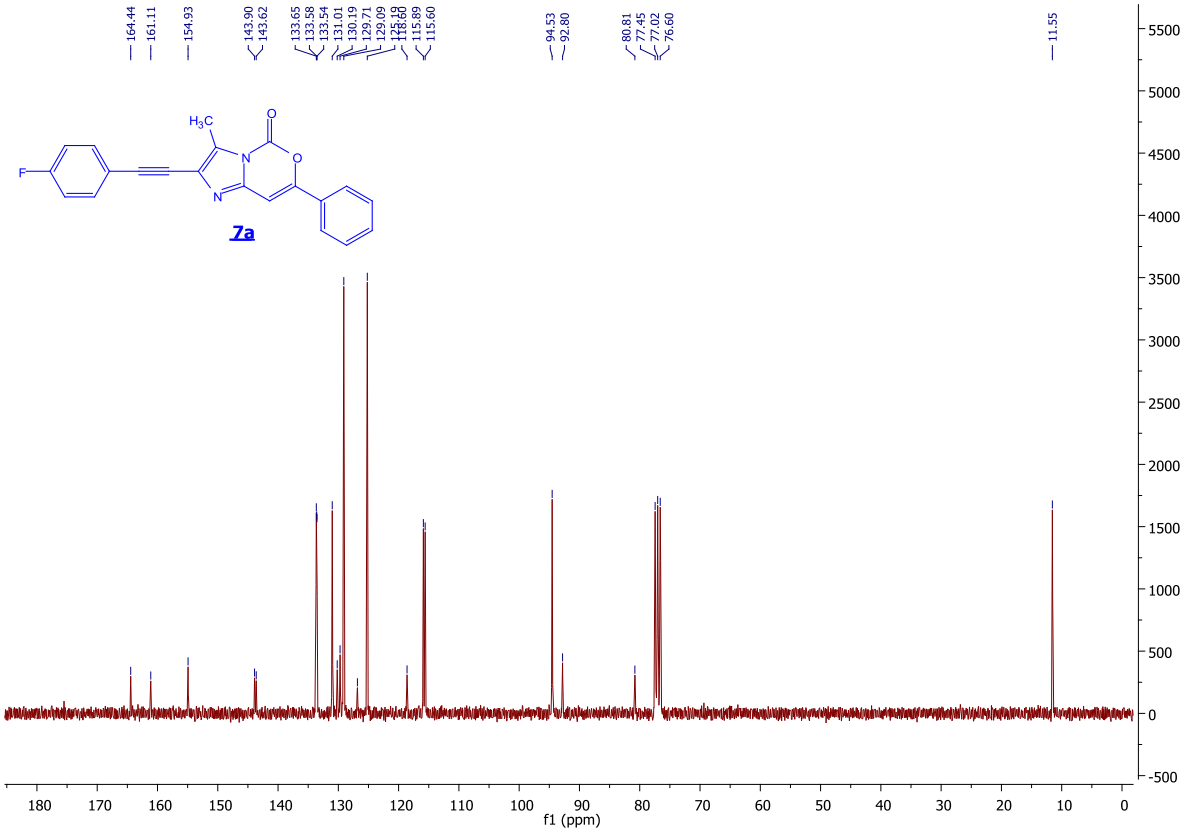
^{1}H NMR (300 MHz, $CDCl_3$) of **7a**



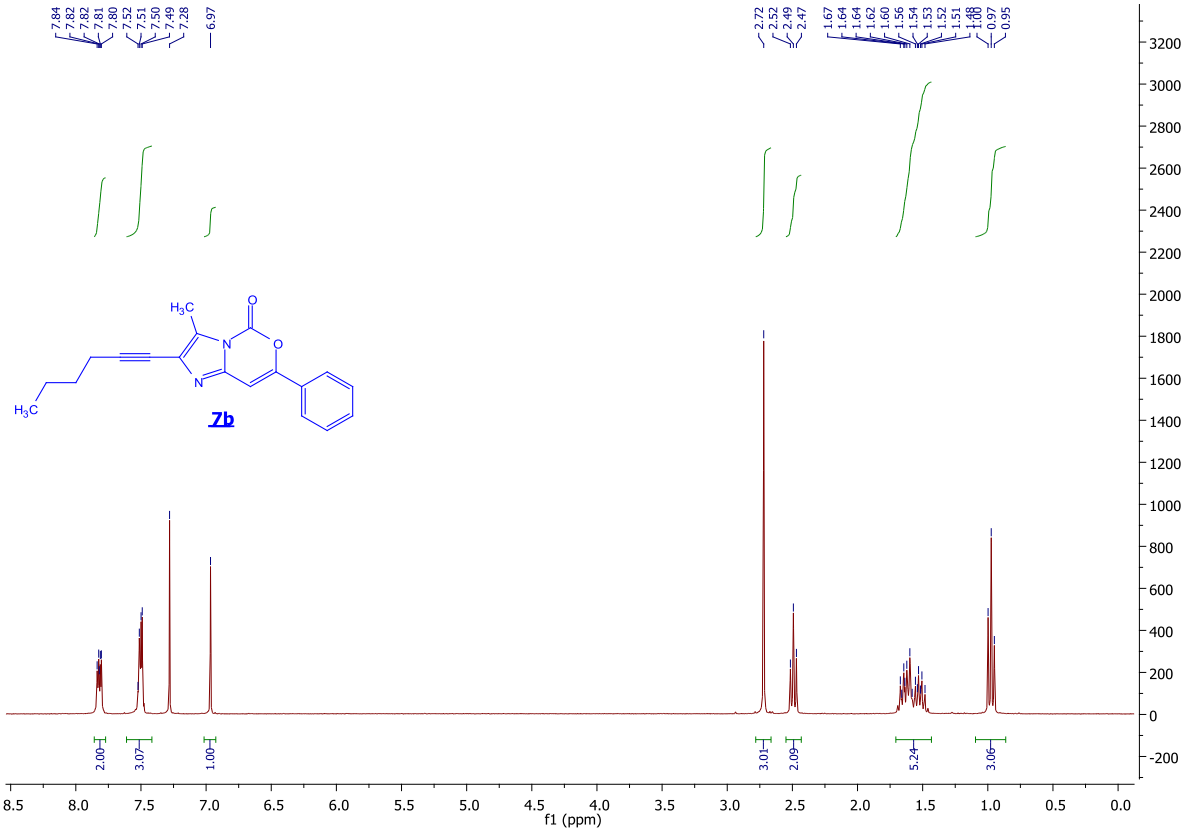
^{19}F NMR (282 MHz, $CDCl_3$) of **7a**



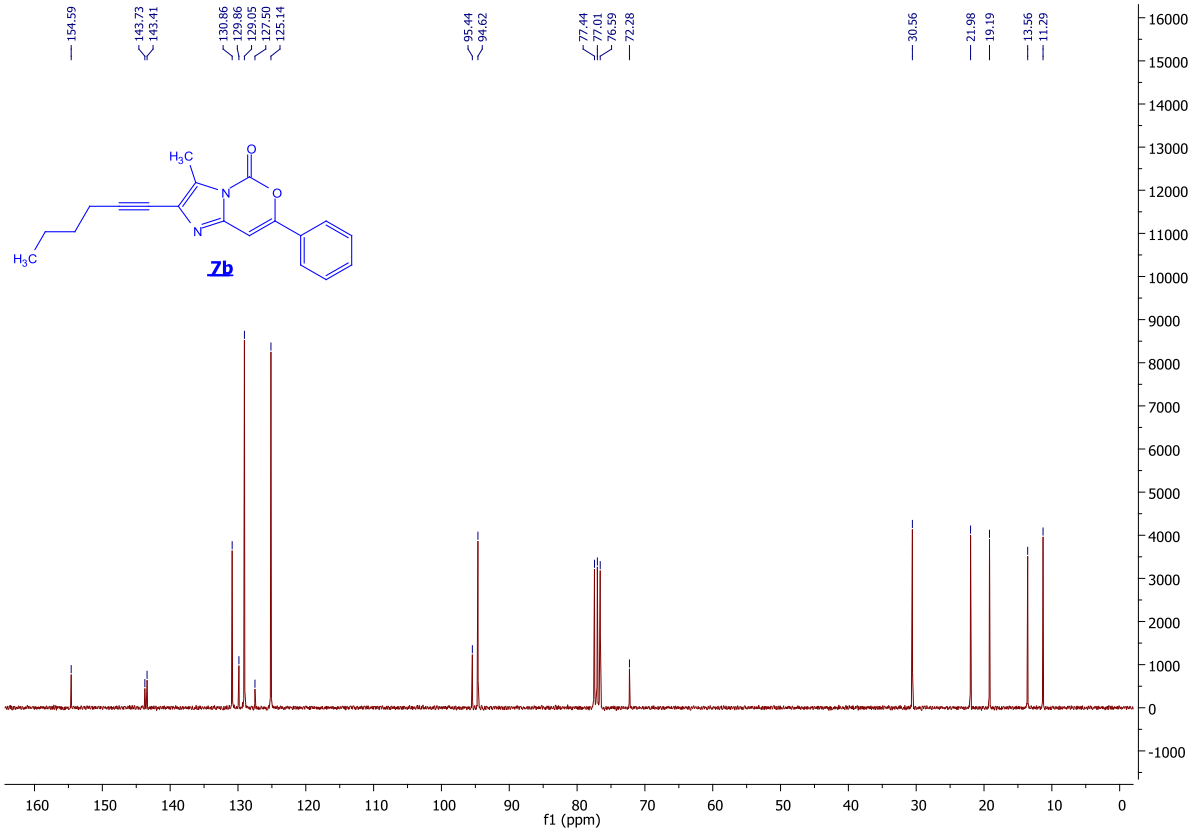
^{13}C NMR (75 MHz, $CDCl_3$) of **7a**



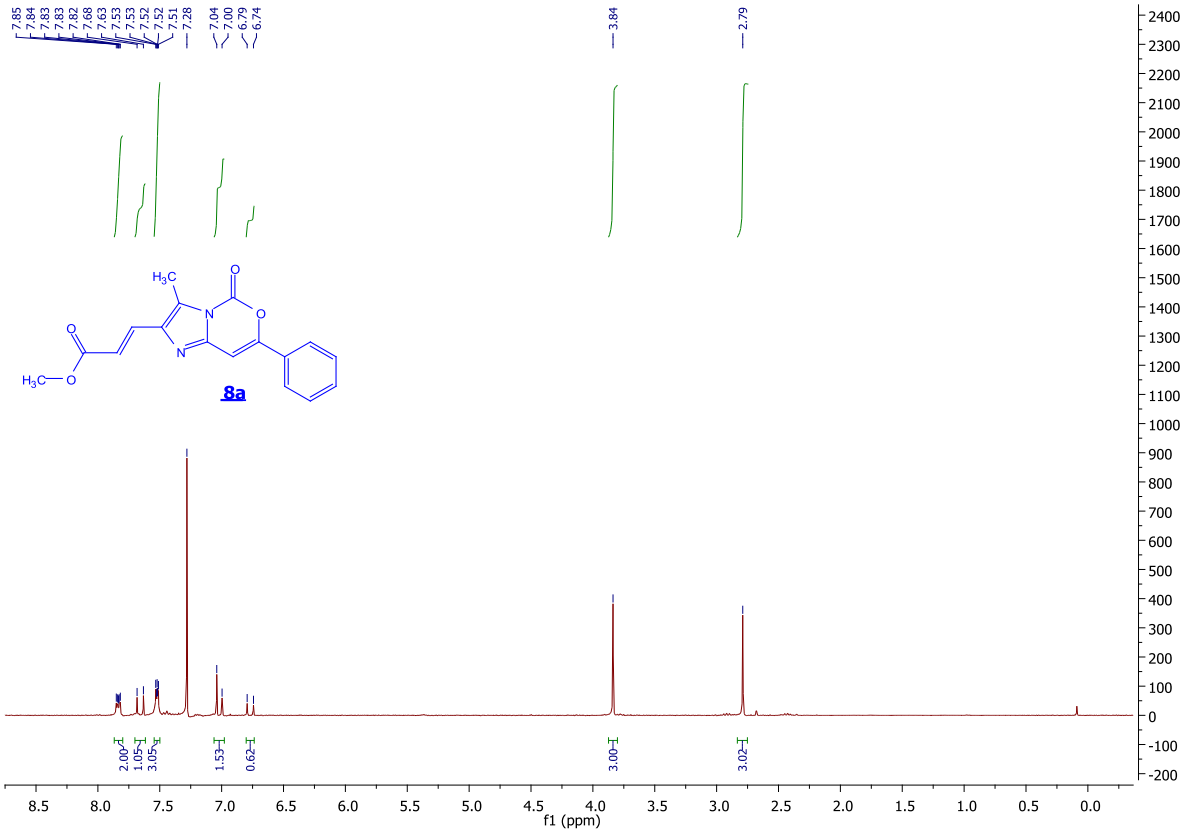
^{1}H NMR (300 MHz, $CDCl_3$) of **7b**



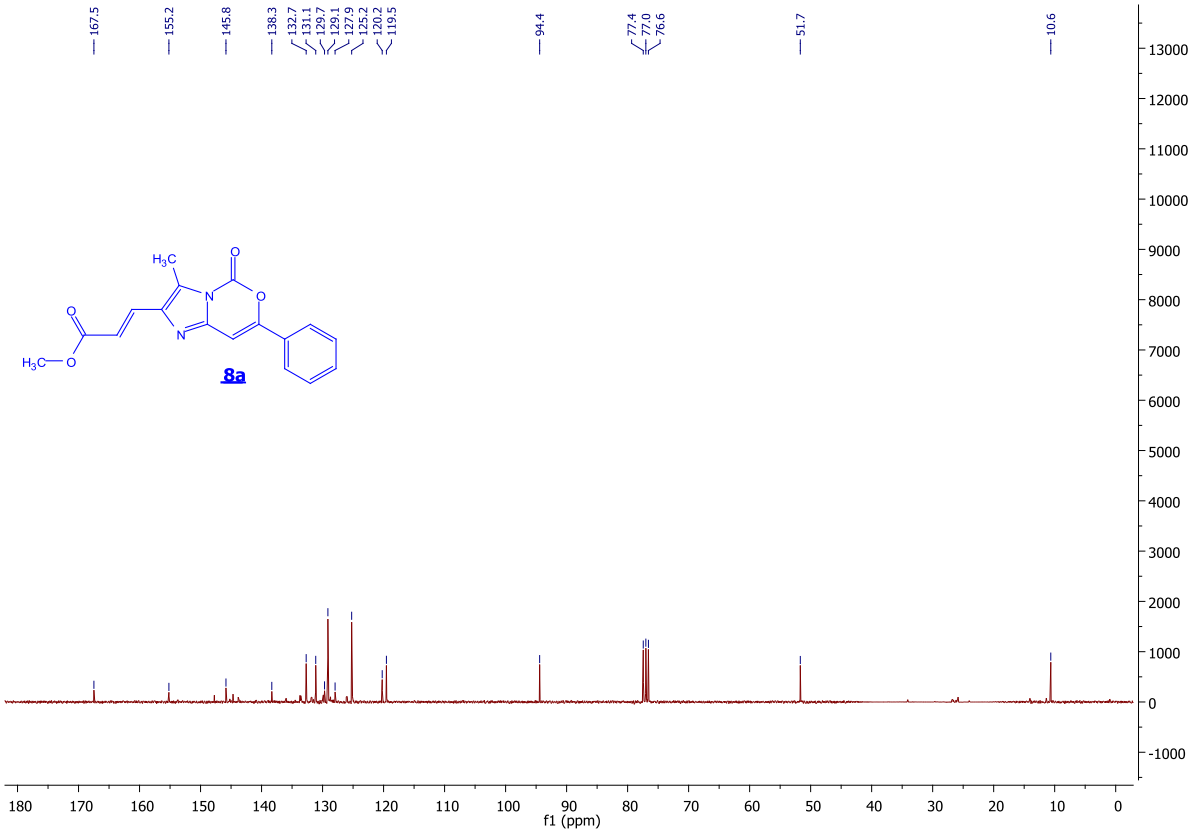
^{13}C NMR (75 MHz, $CDCl_3$) of **7b**



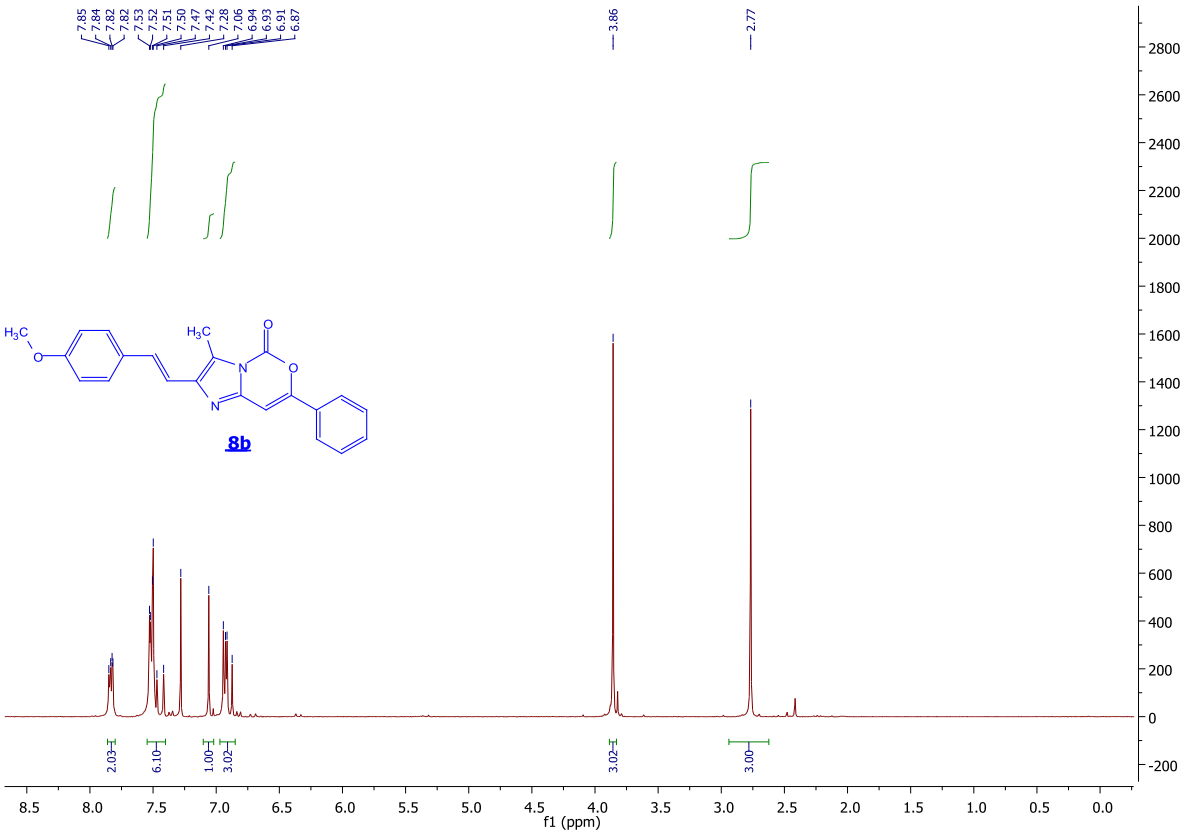
^{1}H NMR (300 MHz, $CDCl_3$) of **8a**



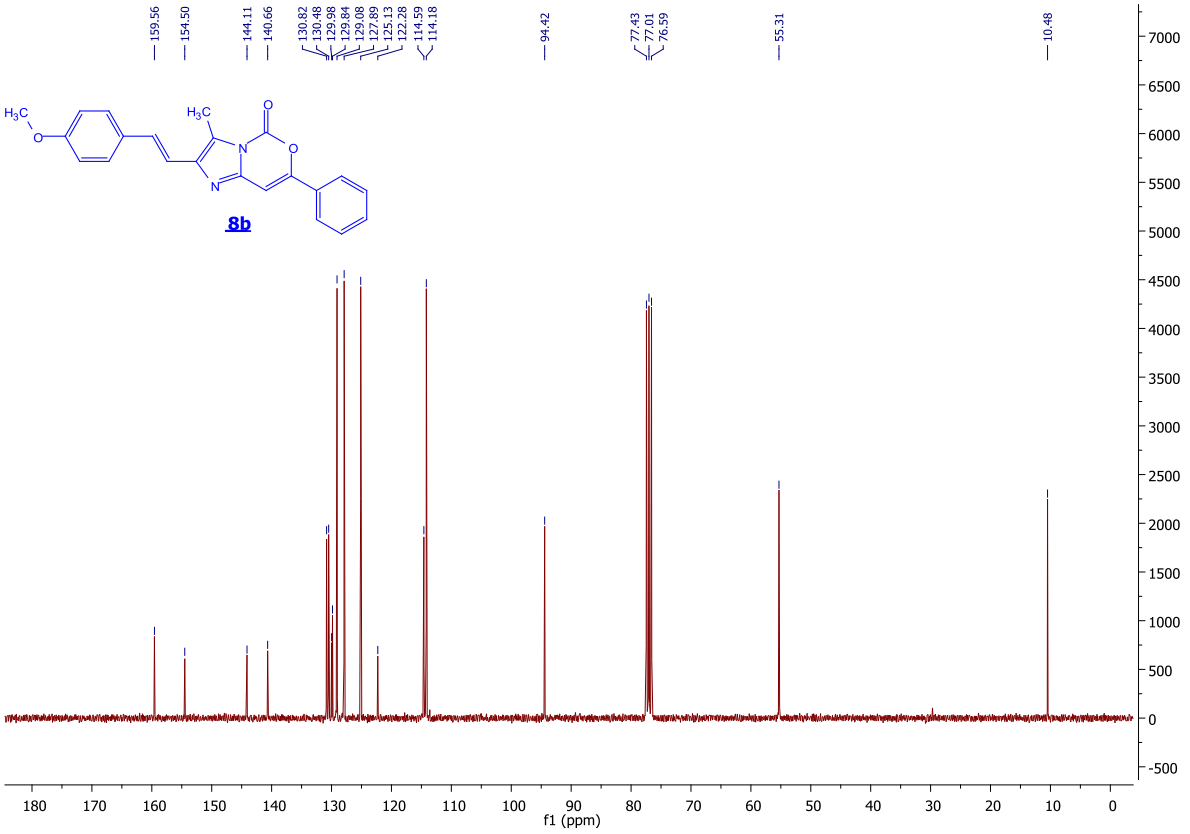
^{13}C NMR (75 MHz, $CDCl_3$) of **8a**



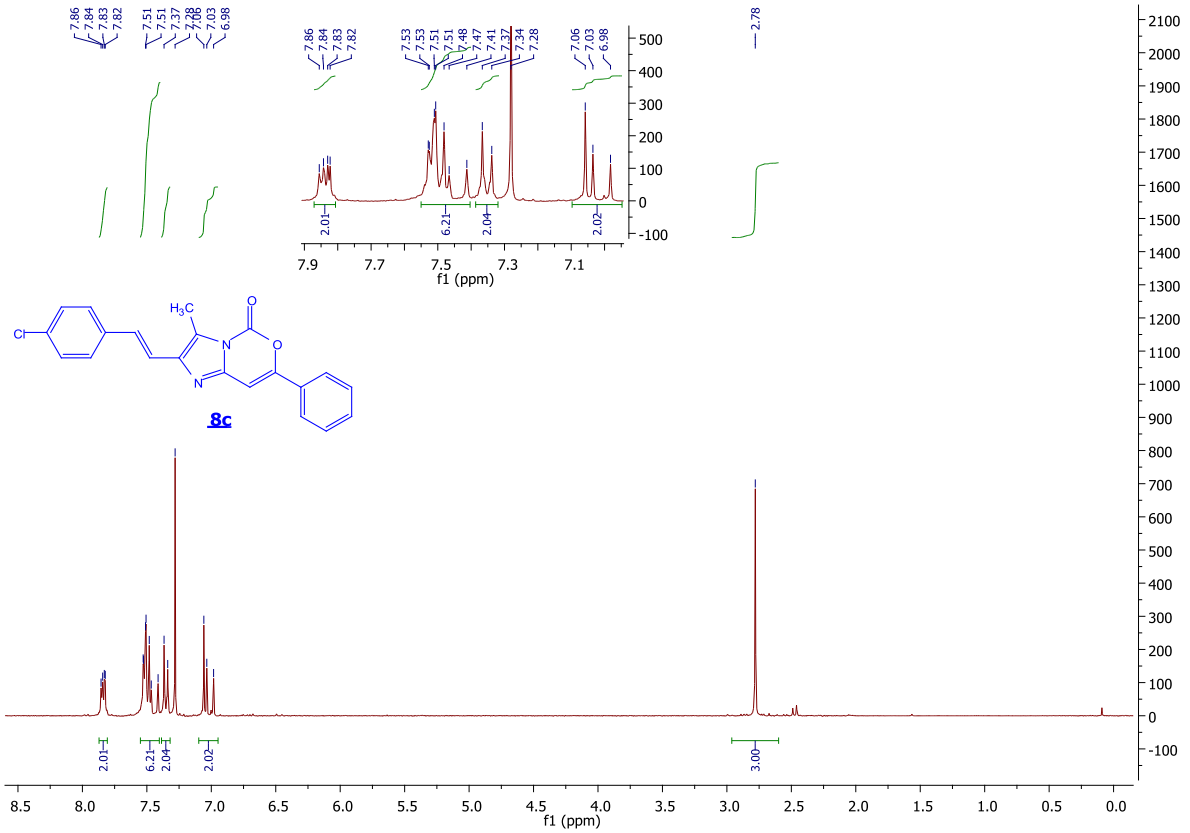
^{1}H NMR (300 MHz, $CDCl_3$) of **8b**



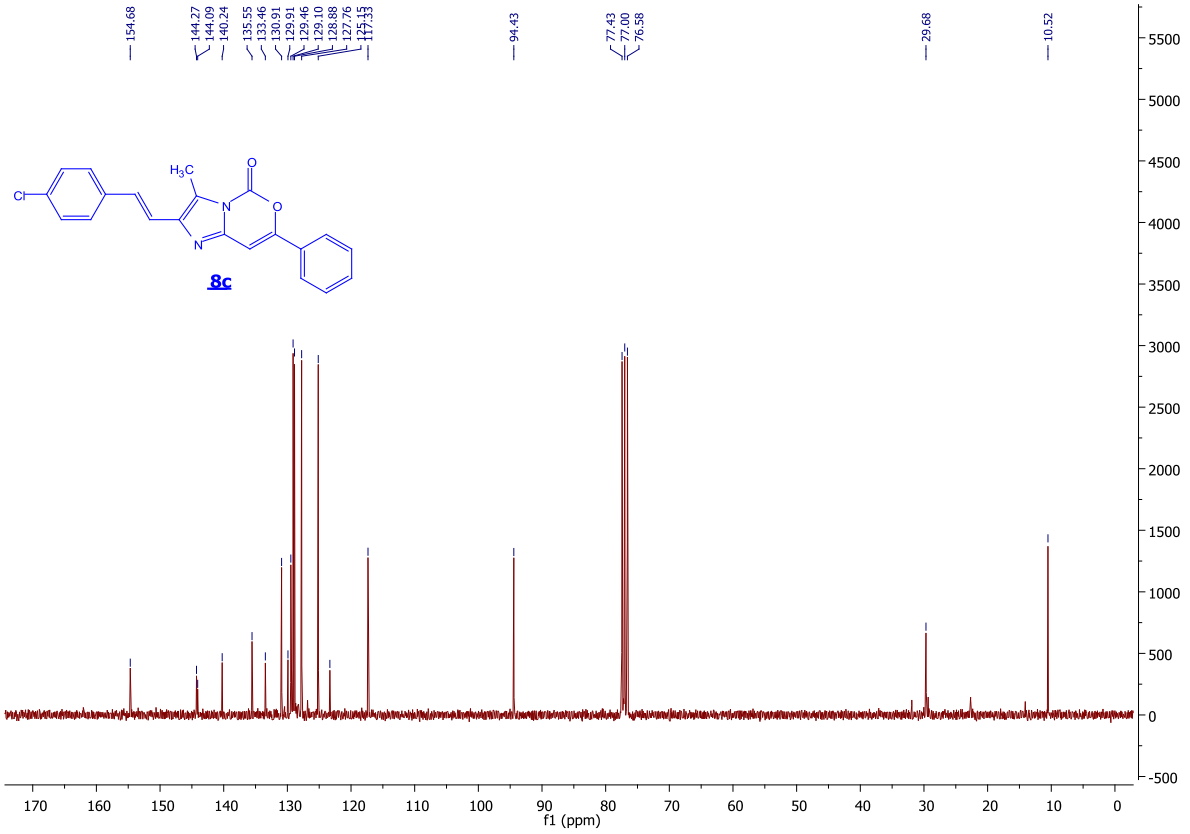
^{13}C NMR (75 MHz, $CDCl_3$) of **8b**



^{1}H NMR (300 MHz, $CDCl_3$) of **8c**



^{13}C NMR (75 MHz, $CDCl_3$) of **8c**



3. Details of DFT calculations

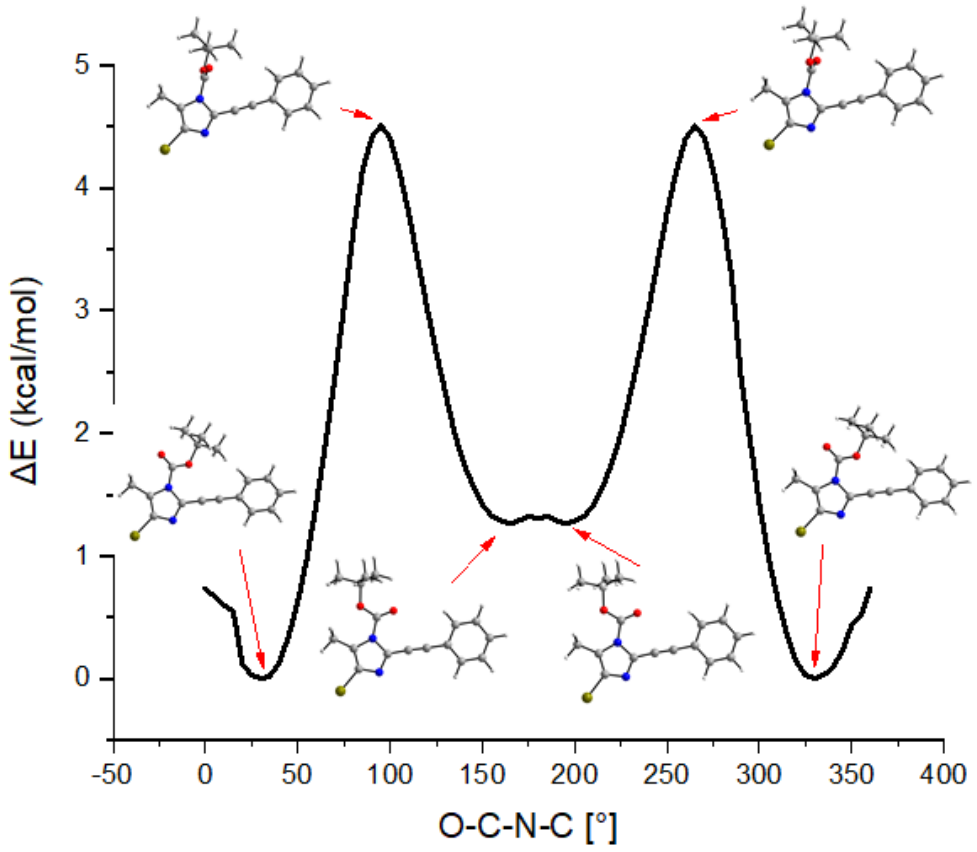


Figure 1: Rotational barrier and conformers of *N*-Boc imidazole **2a**.

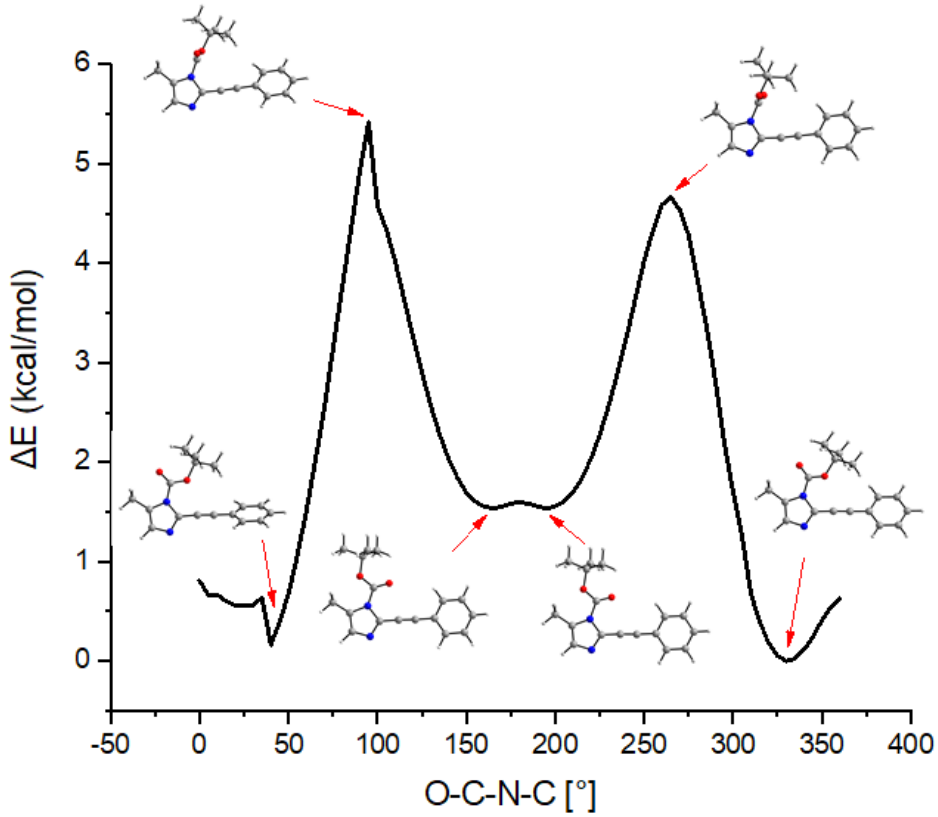


Figure 2: Rotational barrier and conformers of *N*-Boc imidazole **2m**.

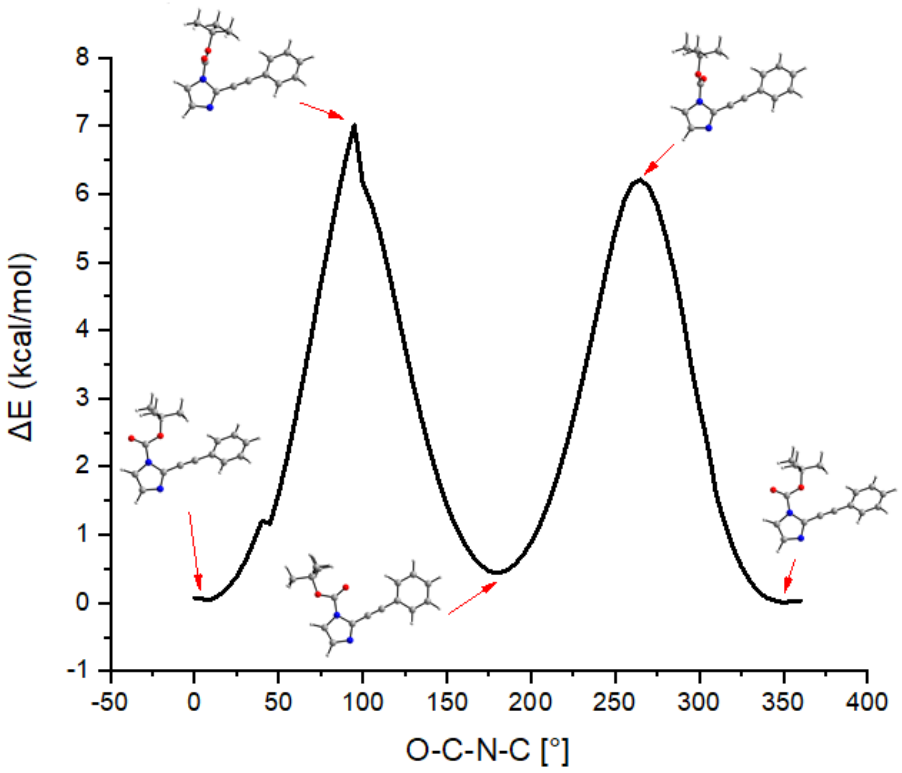


Figure 3: Rotational barrier and conformers of *N*-Boc imidazole **2n**.