Supporting Information

"Synthesis of α-Trifluoromethylthio-α,β-unsaturated Carbonyl Compounds by DABCO-Mediated Electrophilic Trifluoromethylthiolation with *N*-SCF_3-dibenzenesulfonimide"

Jeyeon Yoo,[†] Heun-Jong Ha,[†] Bora Kim, and Chang-Woo Cho*

Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu 41566, Republic of Korea

**E-mail: cwcho@knu.ac.kr*

[†]*J.Y. and H.-J.H. contributed equally to this work.*

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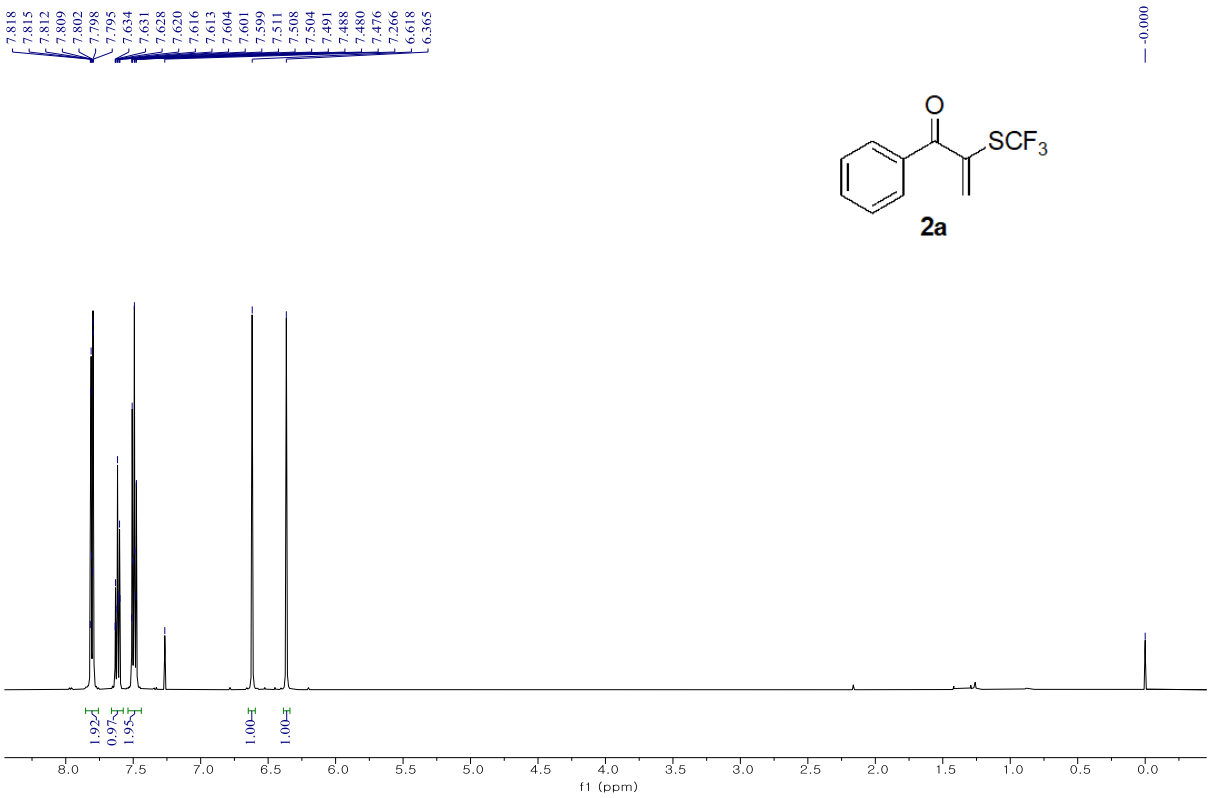
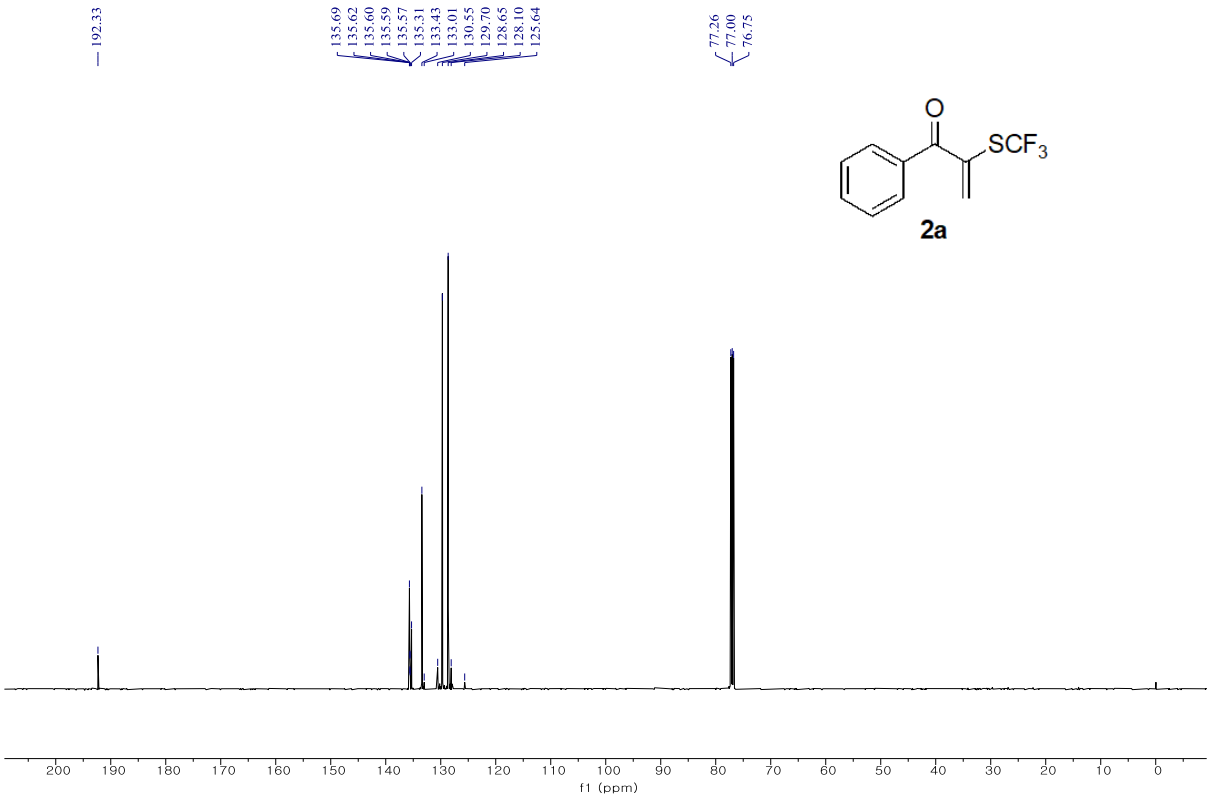
*[1]H NMR of **2a** (500 MHz, $CDCl_3$)*

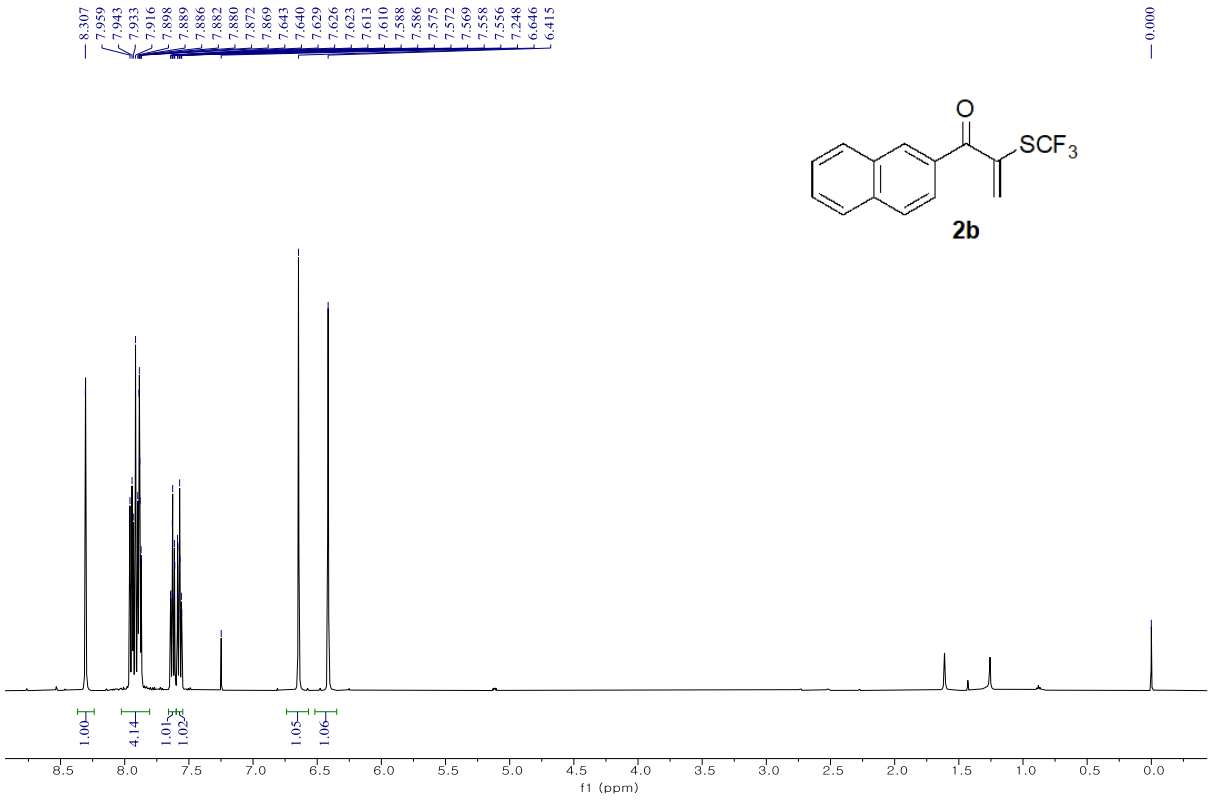


*[13]C NMR of **2a** (125 MHz, $CDCl_3$)*



*^{19}F NMR of **2a** (564 MHz, $CDCl_3$)*

*^{1}H NMR of **2b** (500 MHz, $CDCl_3$)*



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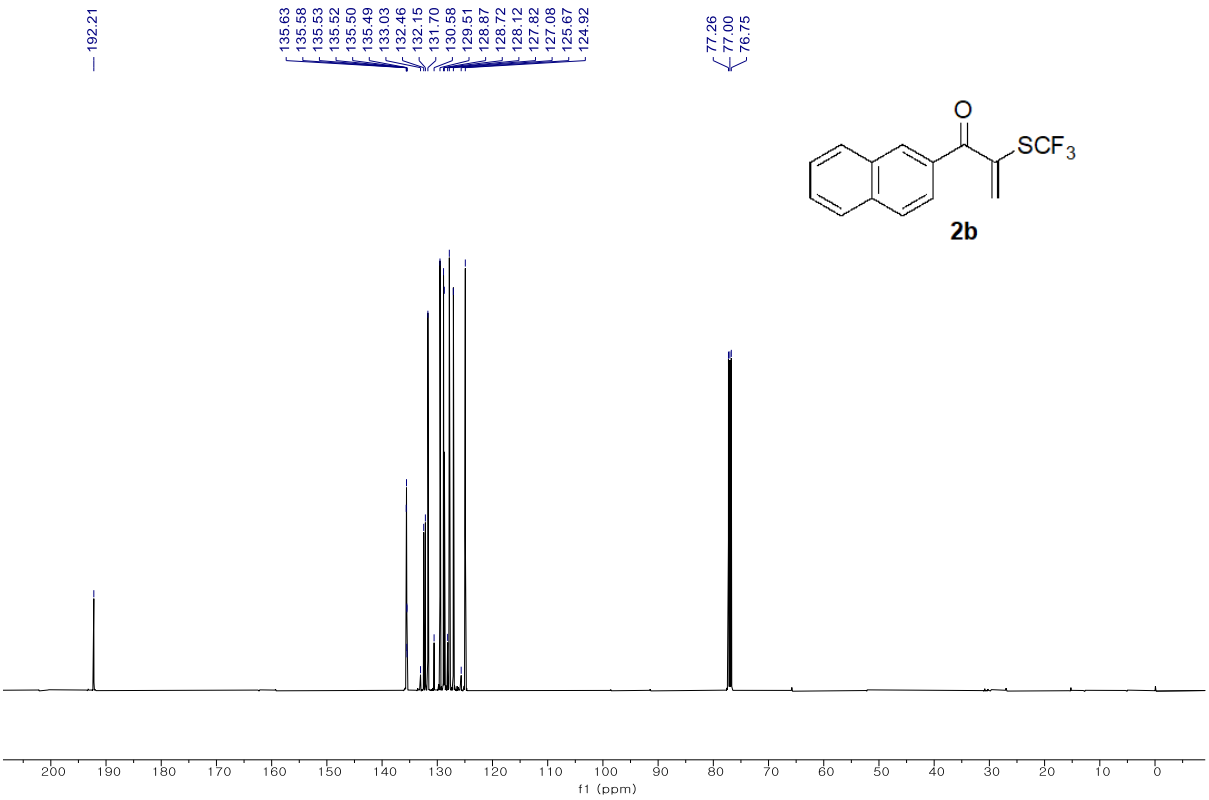

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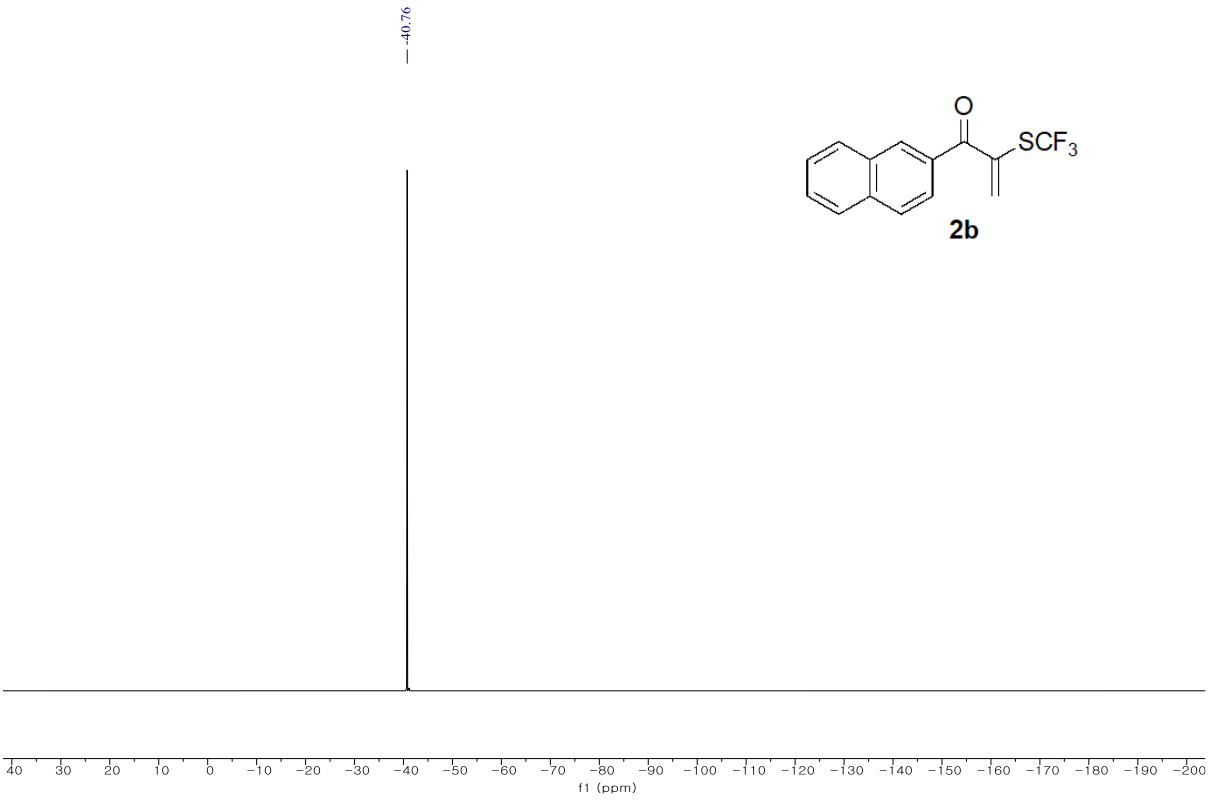

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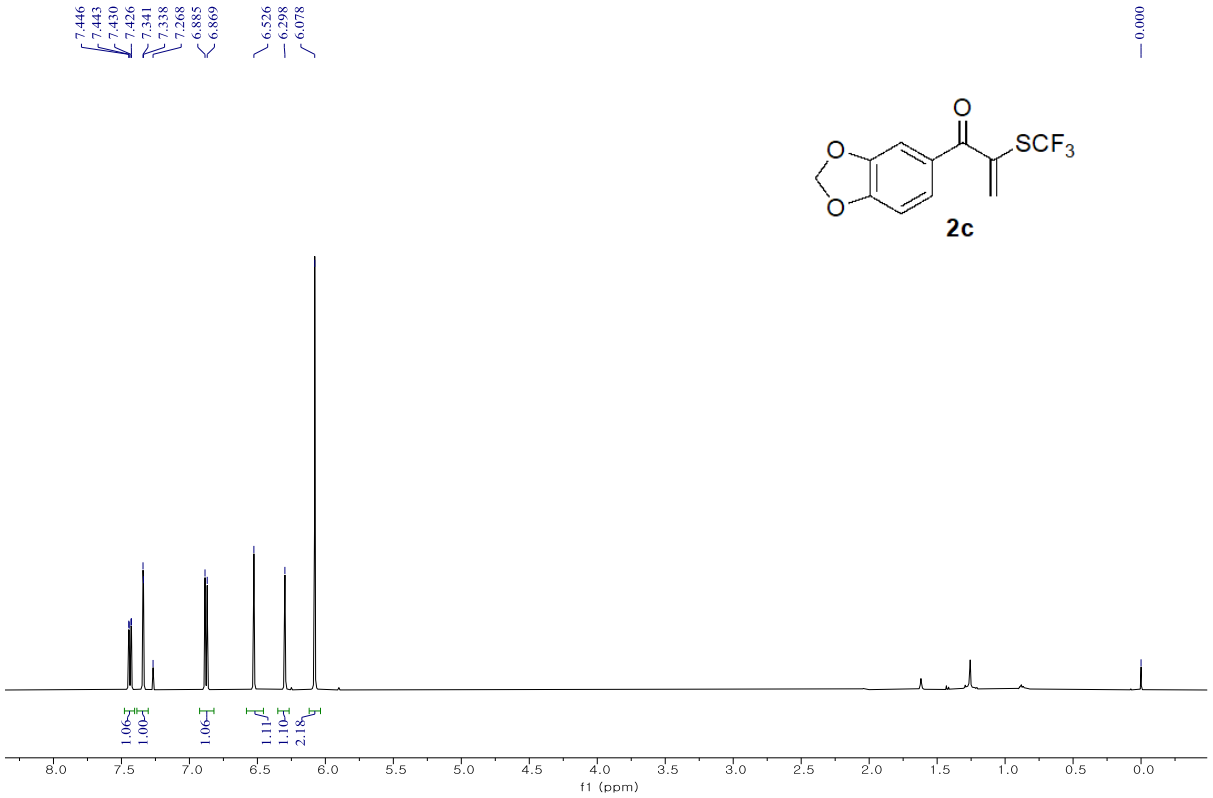

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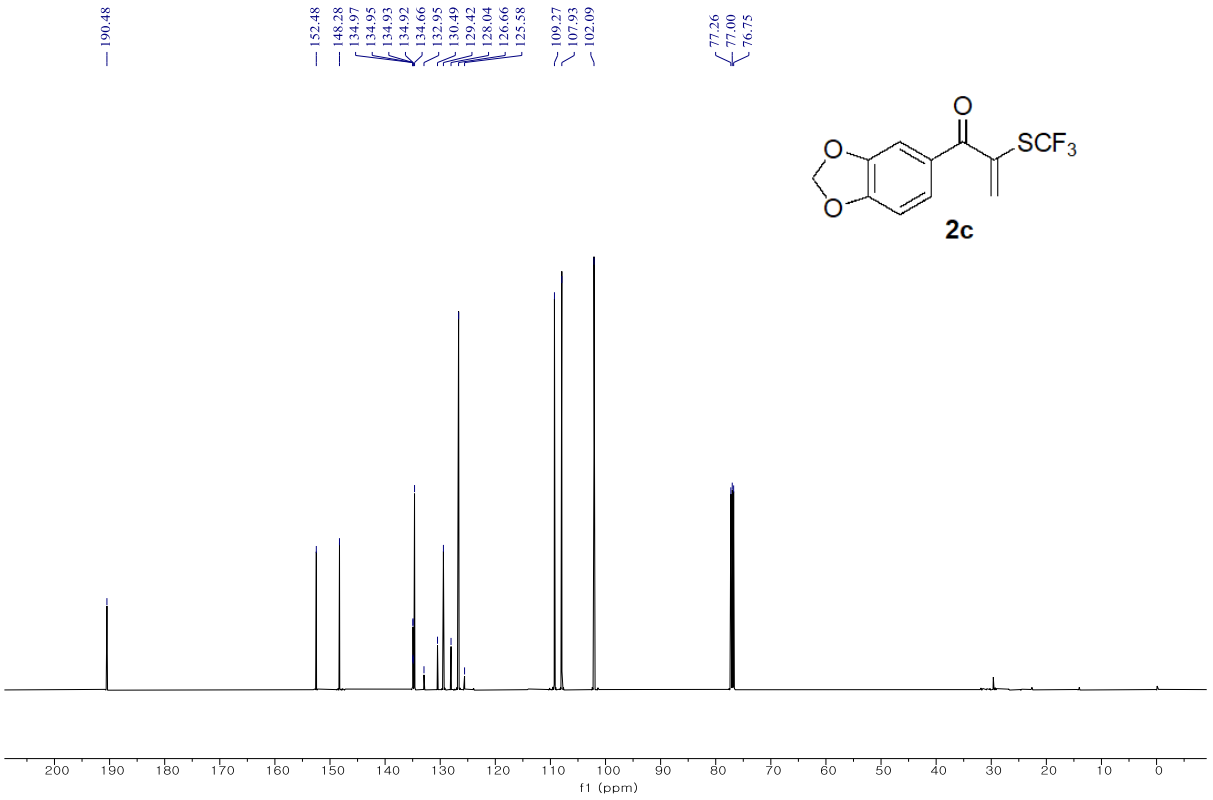
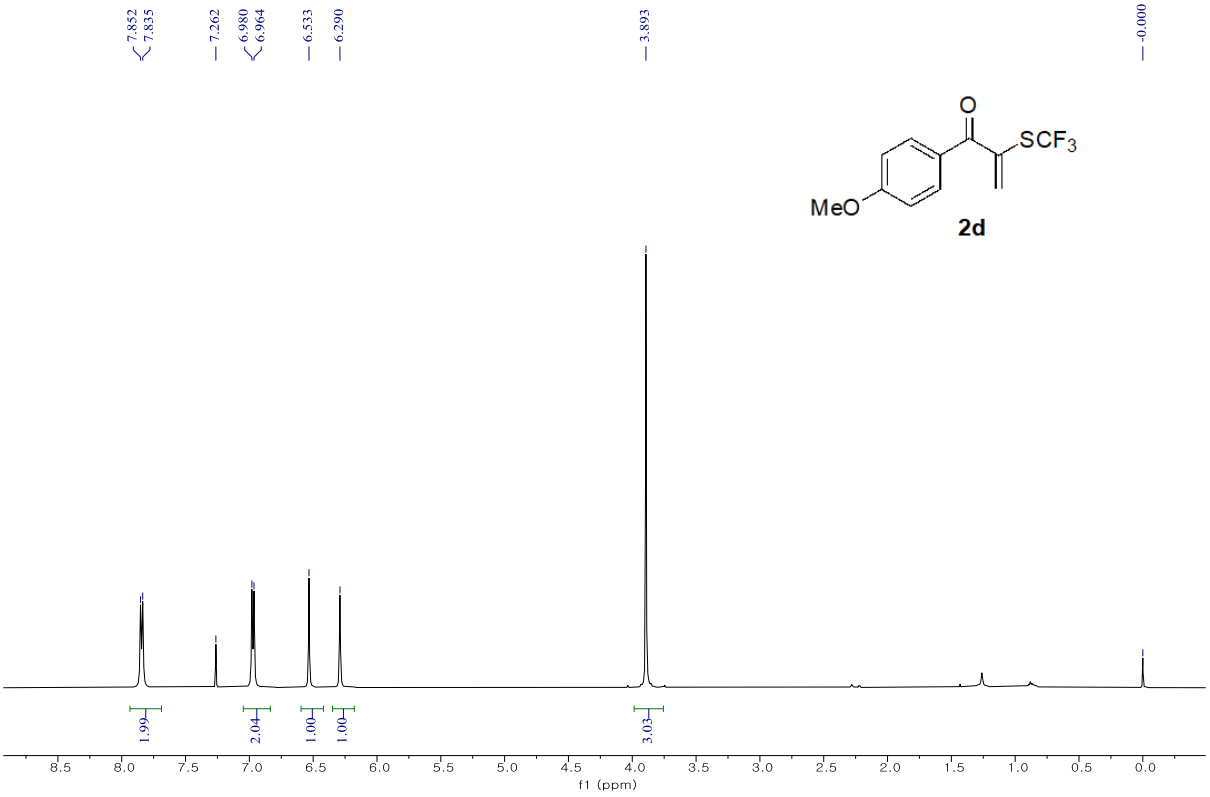


*^{19}F NMR of **2c** (564 MHz, $CDCl_3$)*

*^{1}H NMR of **2d** (500 MHz, $CDCl_3$)*



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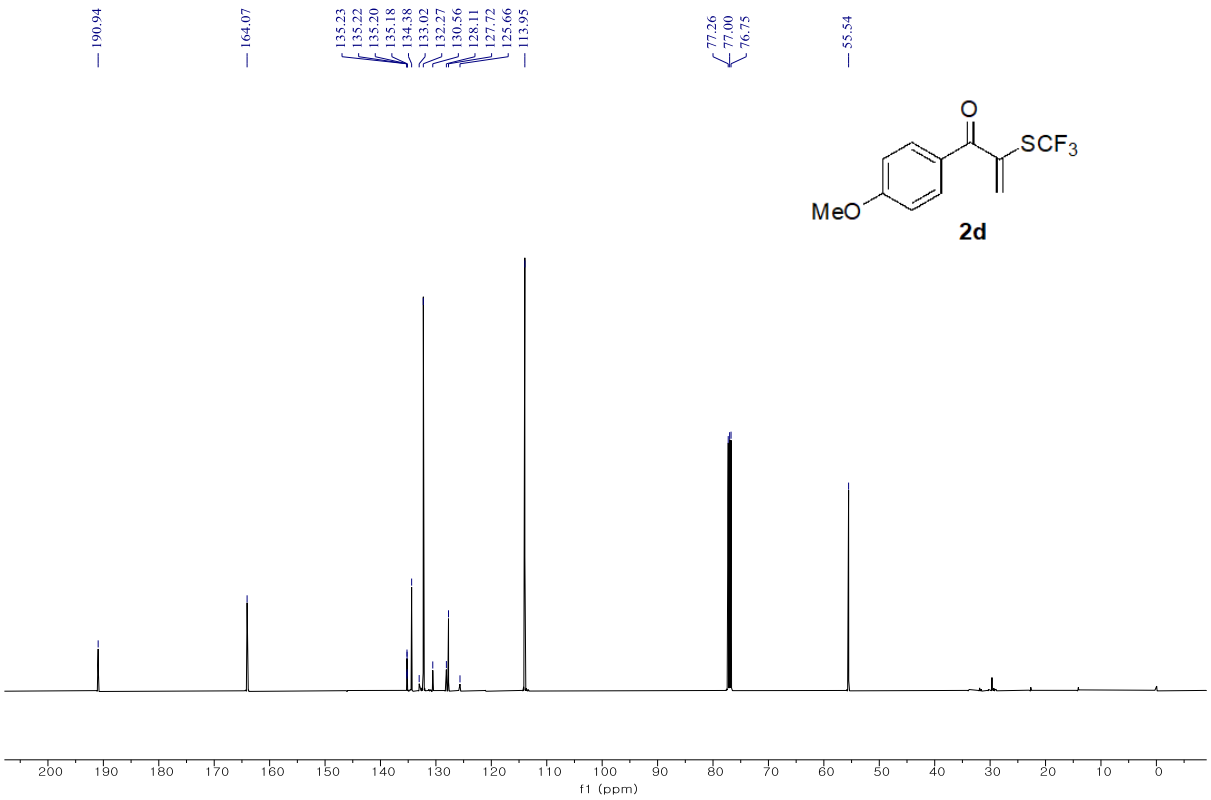

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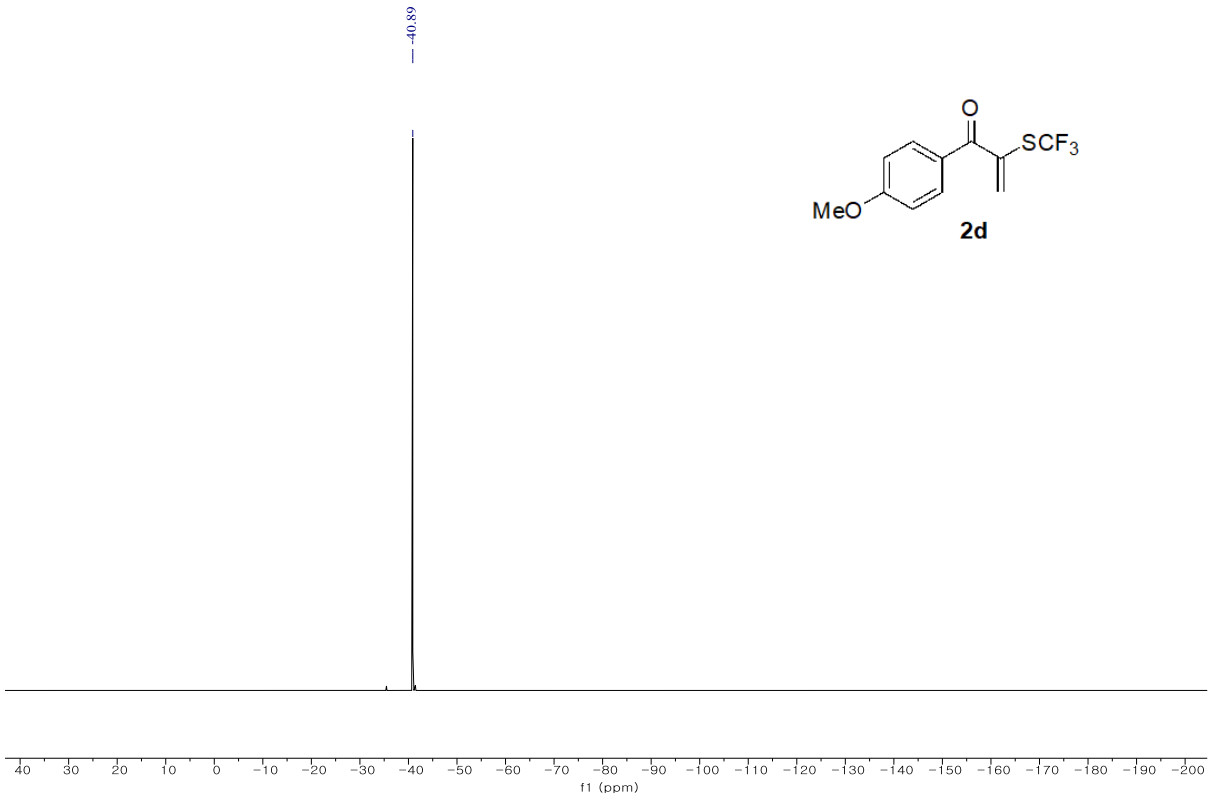

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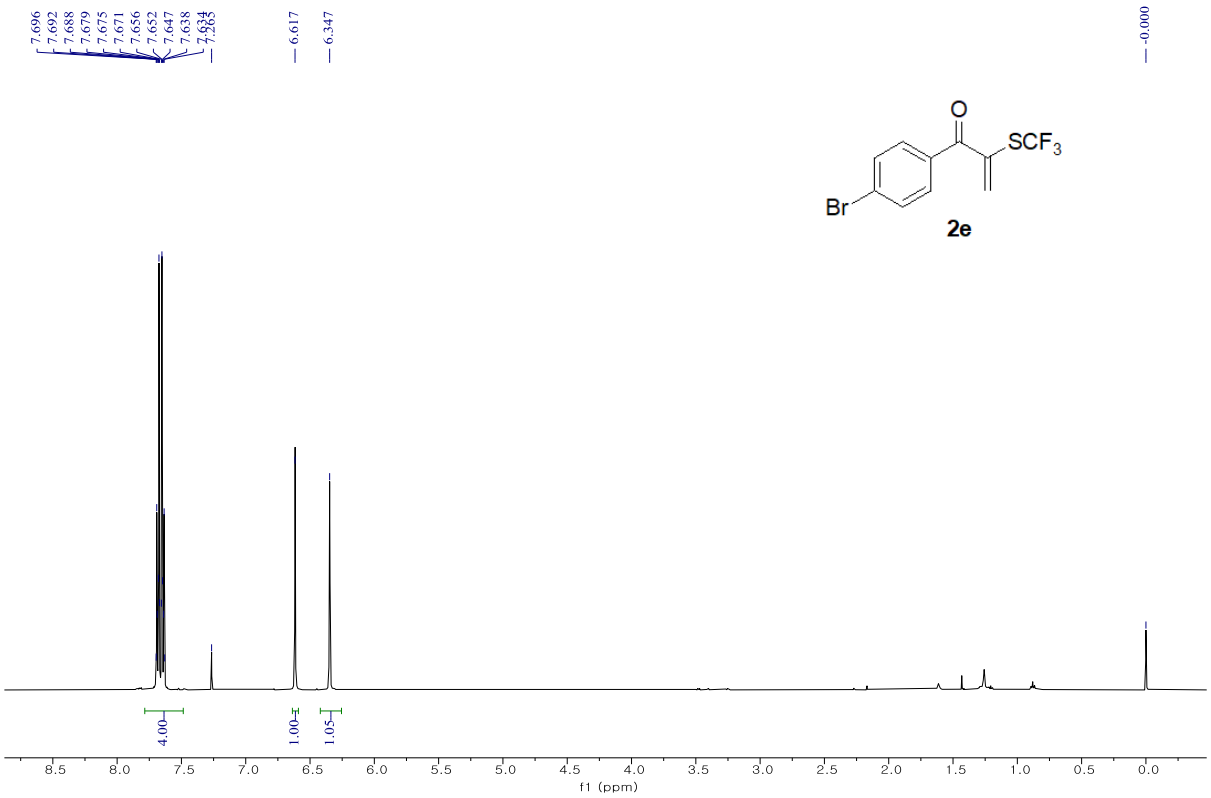
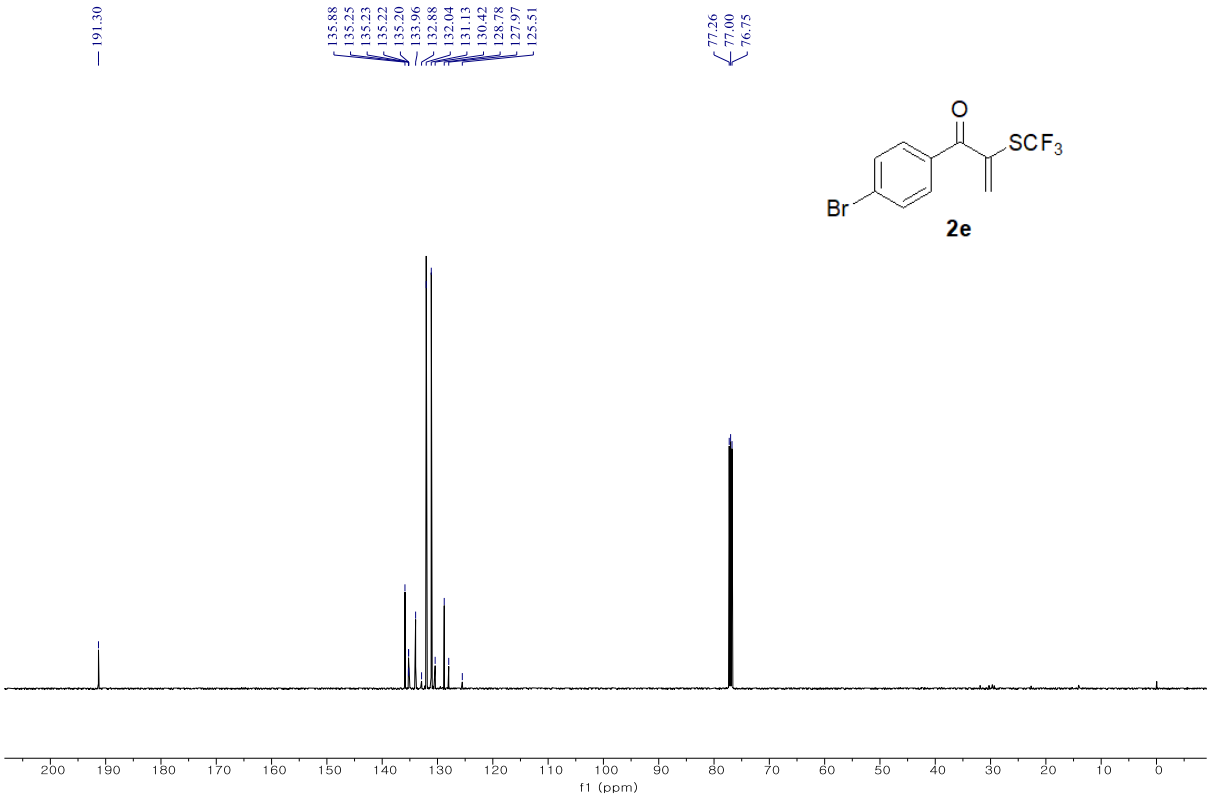
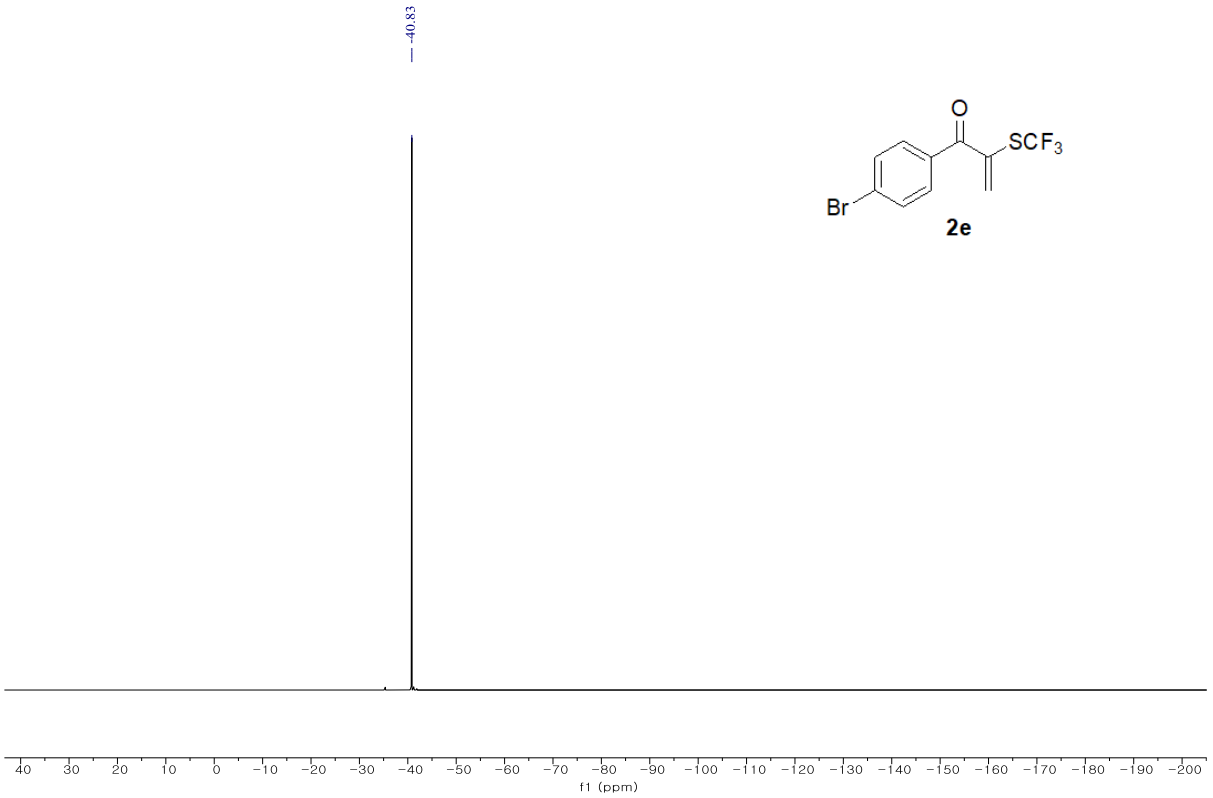


*[13]C NMR of **2e** (125 MHz, CDCl3)*



*^{19}F NMR of **2e** (564 MHz, $CDCl_3$)*



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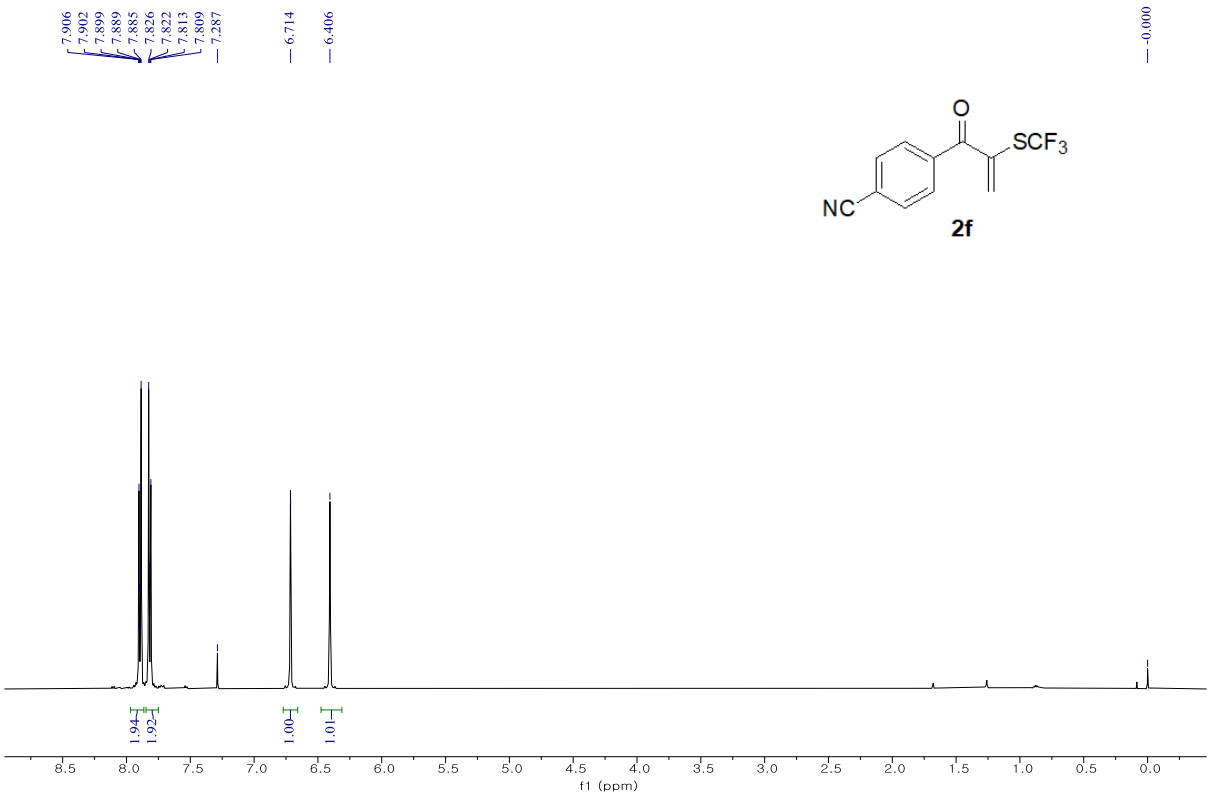
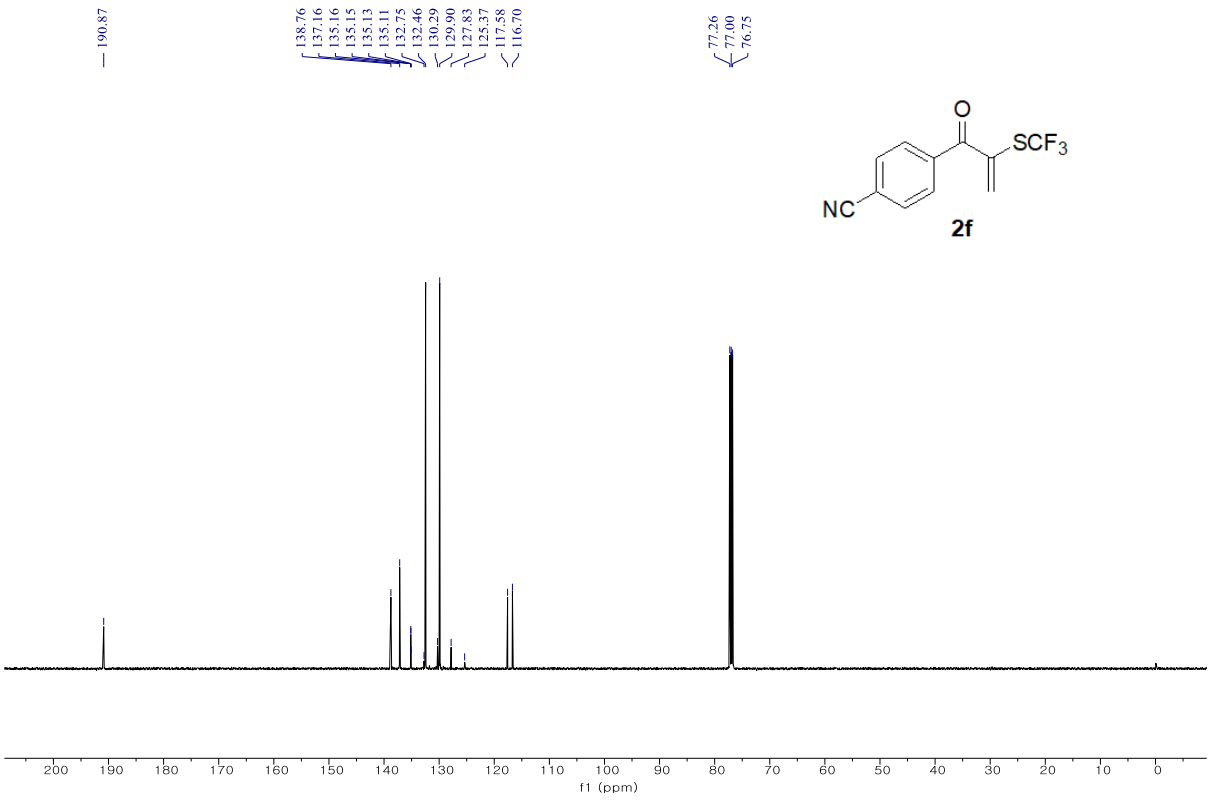
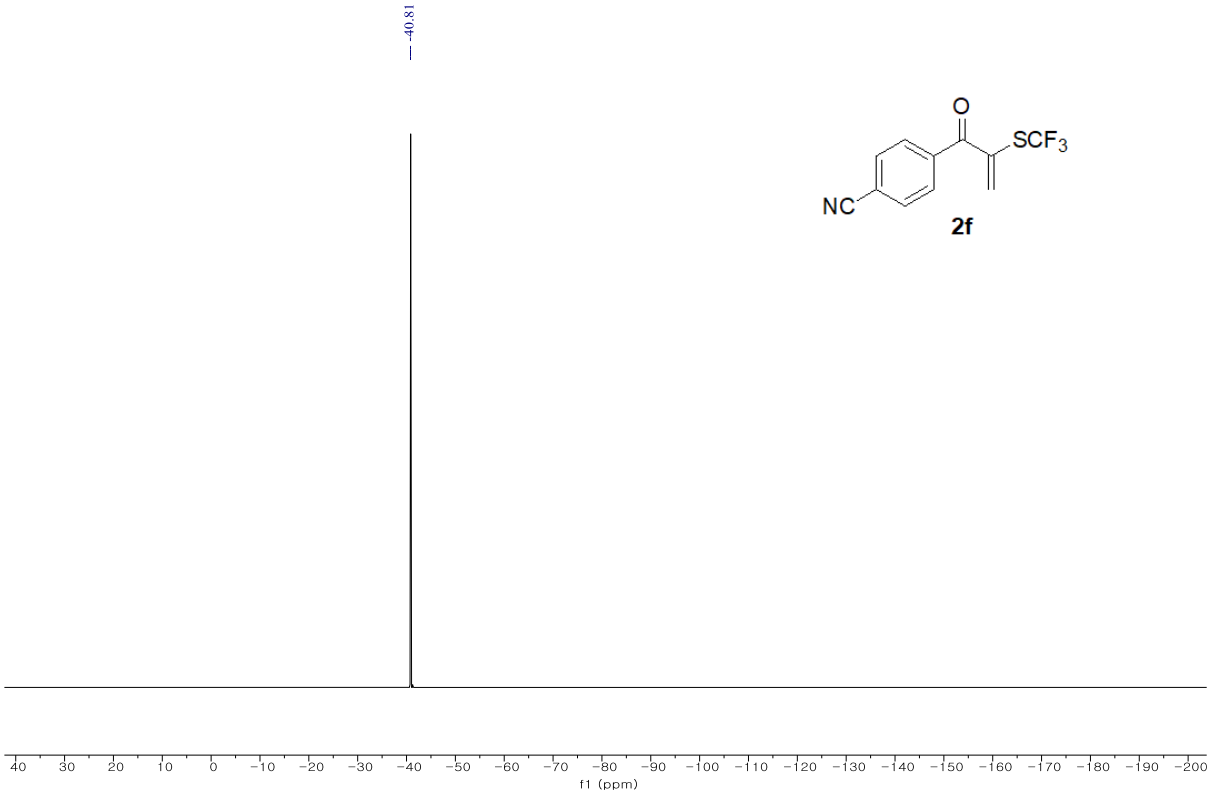


*^{13}C NMR of **2f** (125 MHz, $CDCl_3$)*



*^{19}F NMR of **2f** (564 MHz, $CDCl_3$)*



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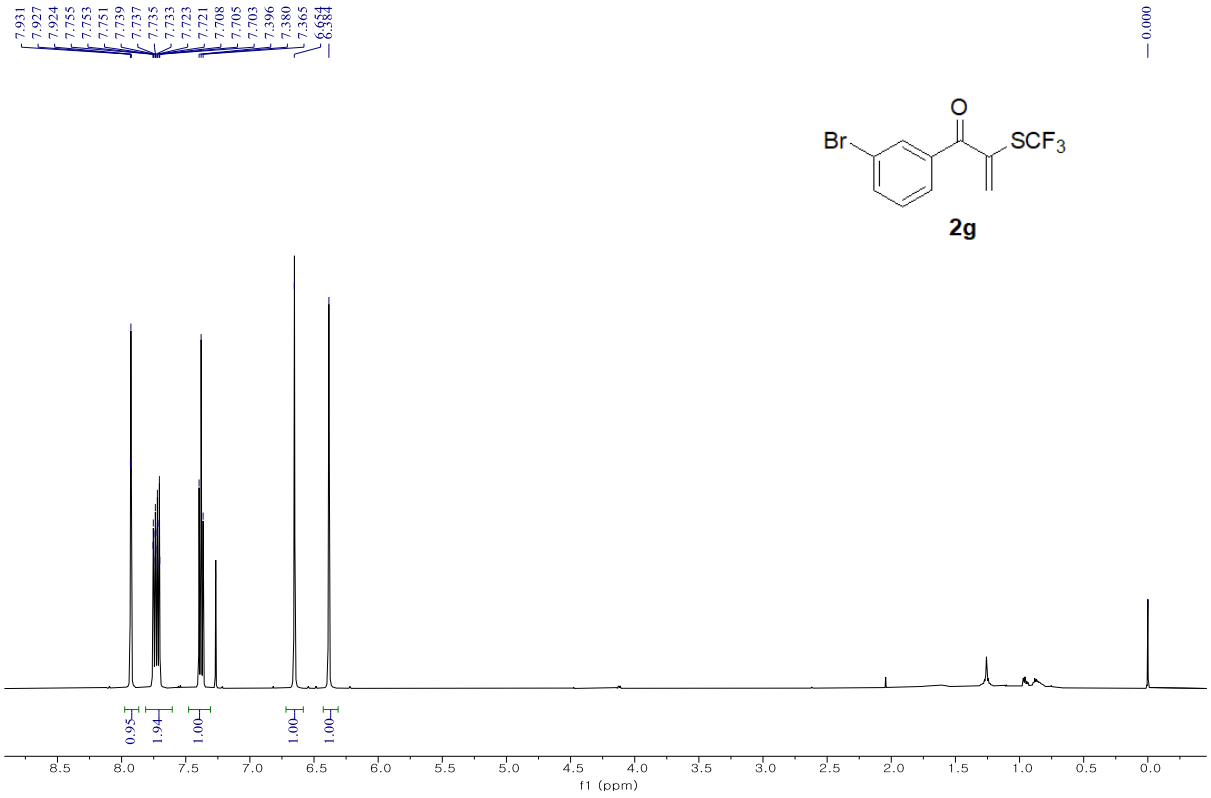

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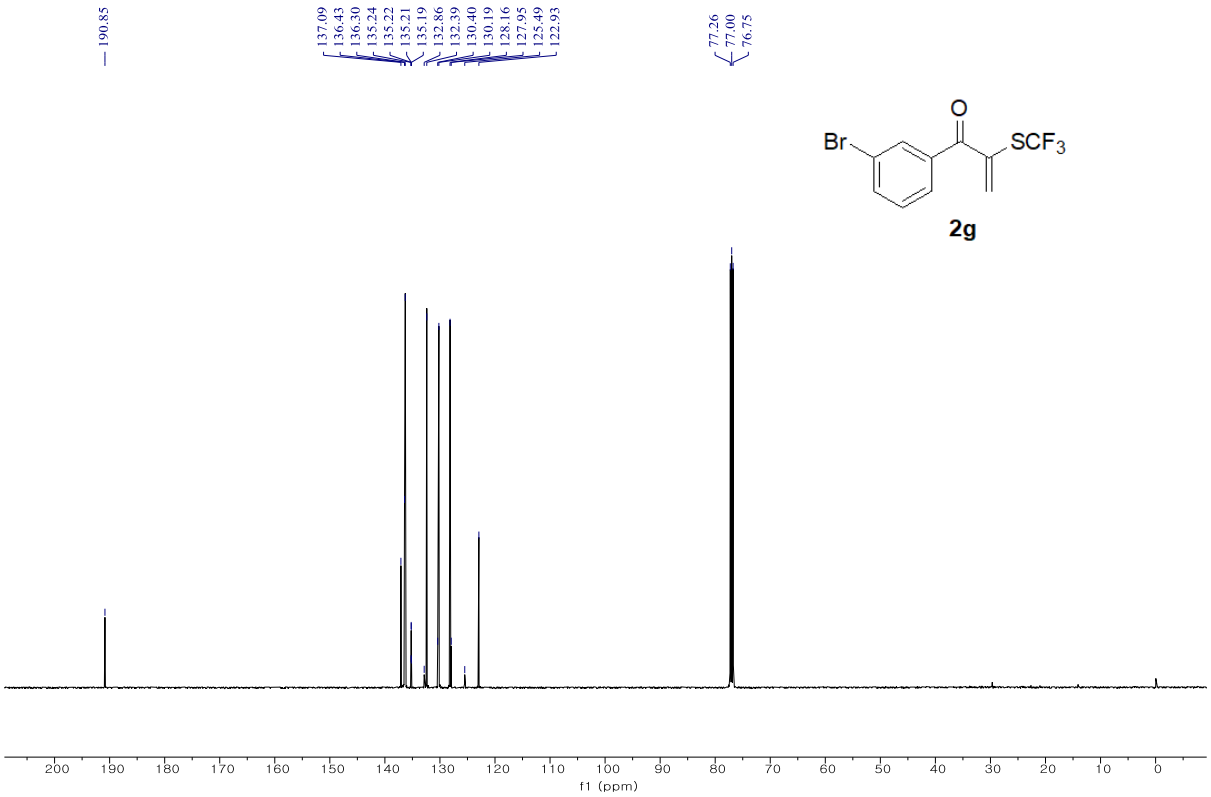
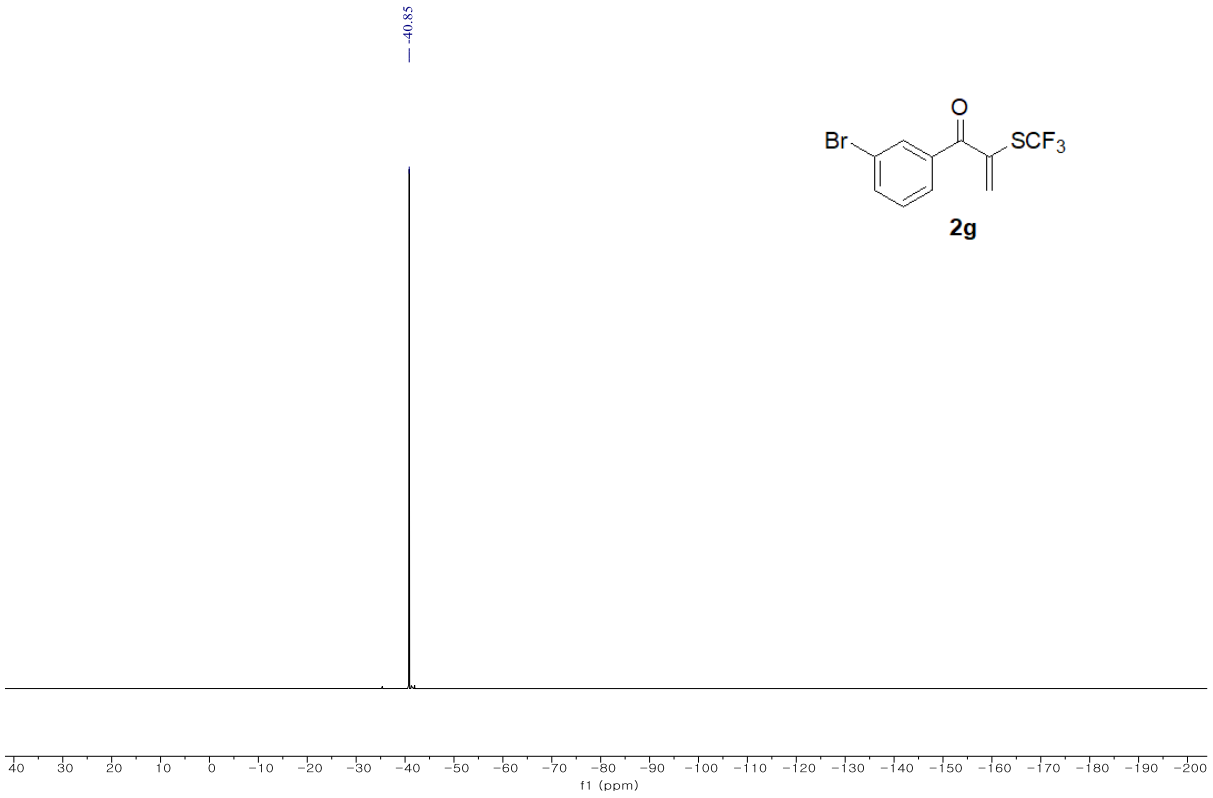


*^{19}F NMR of **2g** (564 MHz, $CDCl_3$)*



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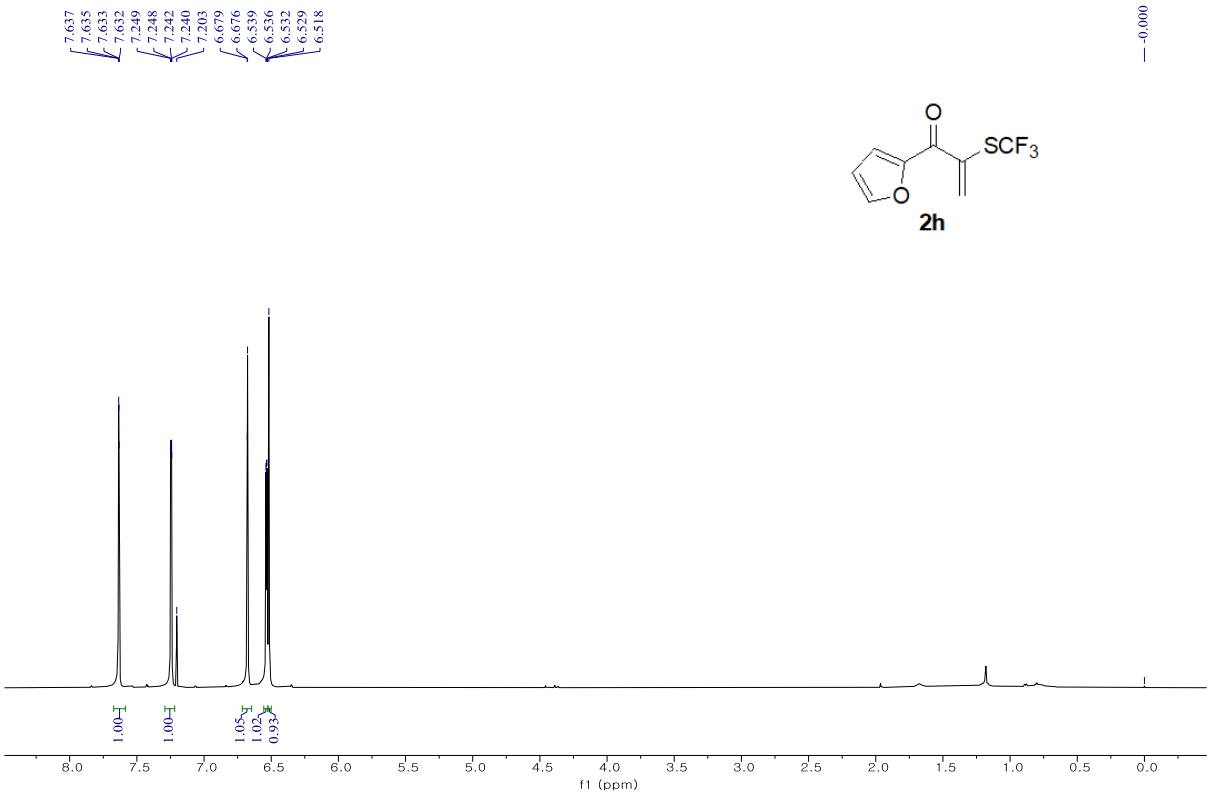
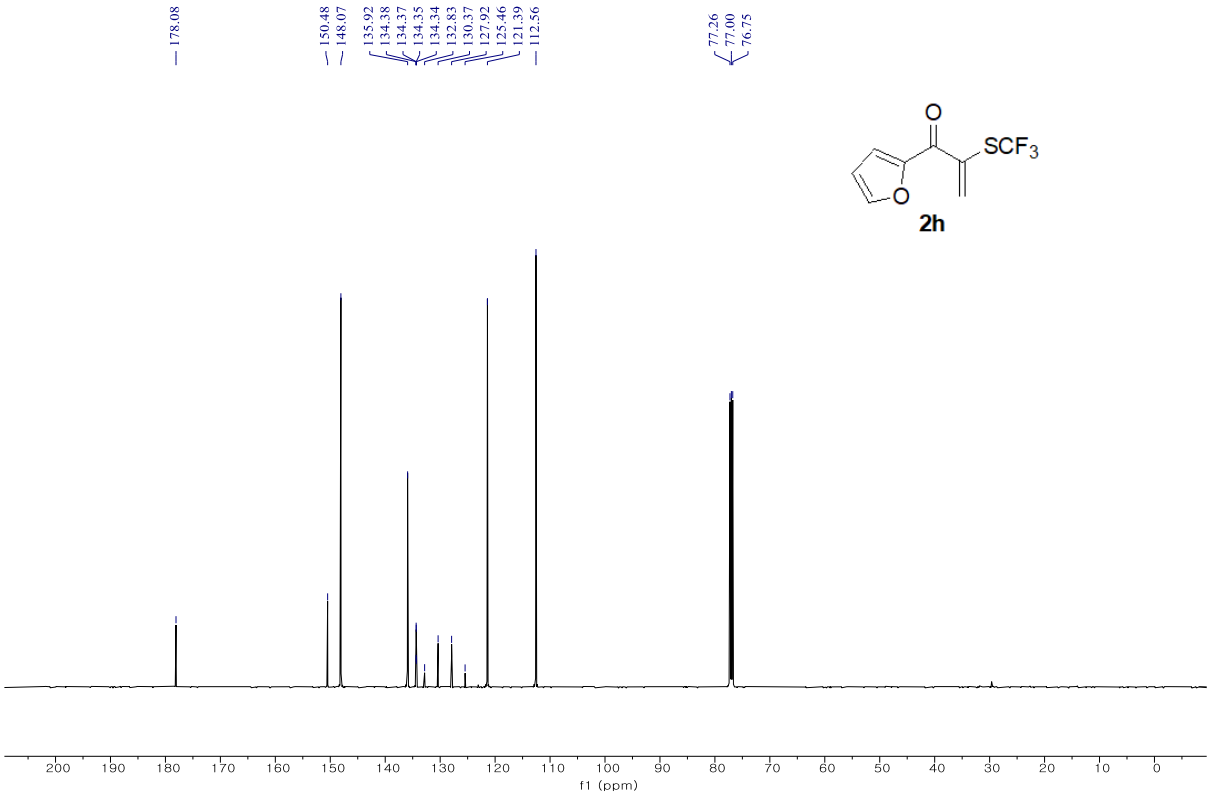
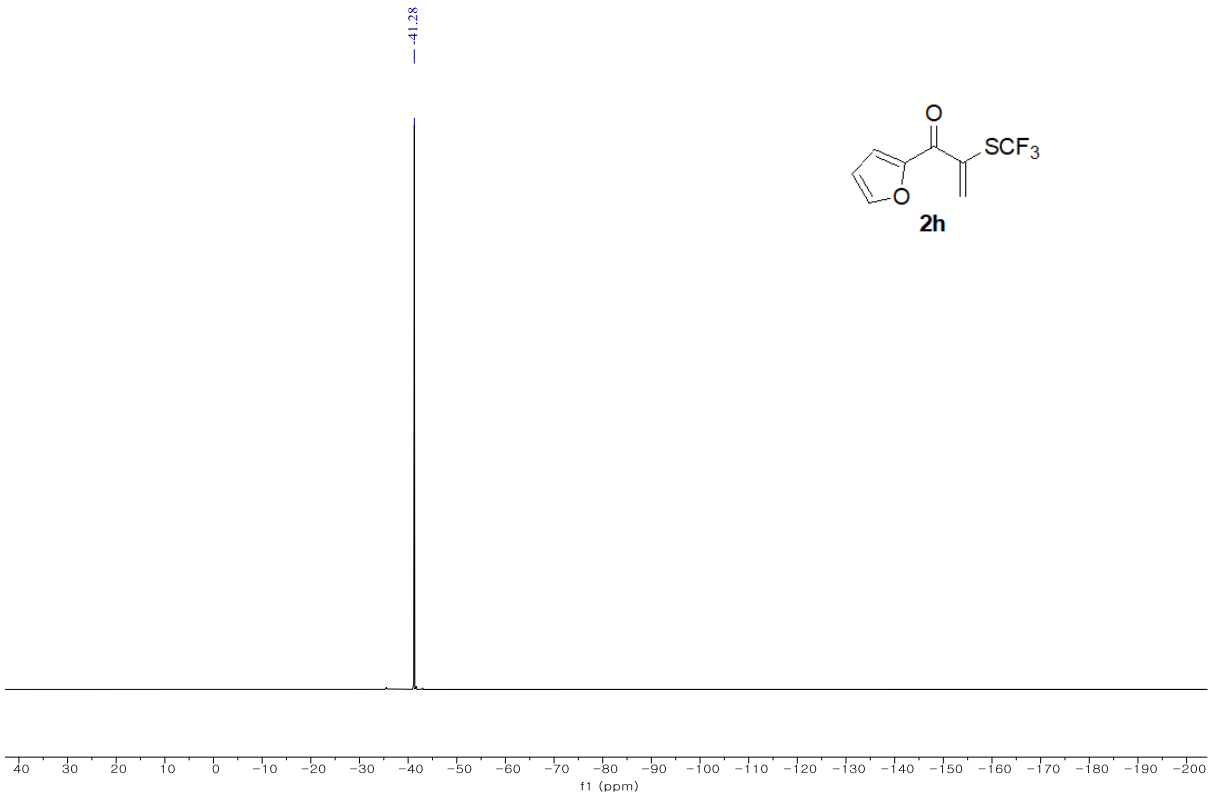


*^{13}C NMR of **2h** (125 MHz, $CDCl_3$)*



*^{19}F NMR of **2h** (564 MHz, $CDCl_3$)*



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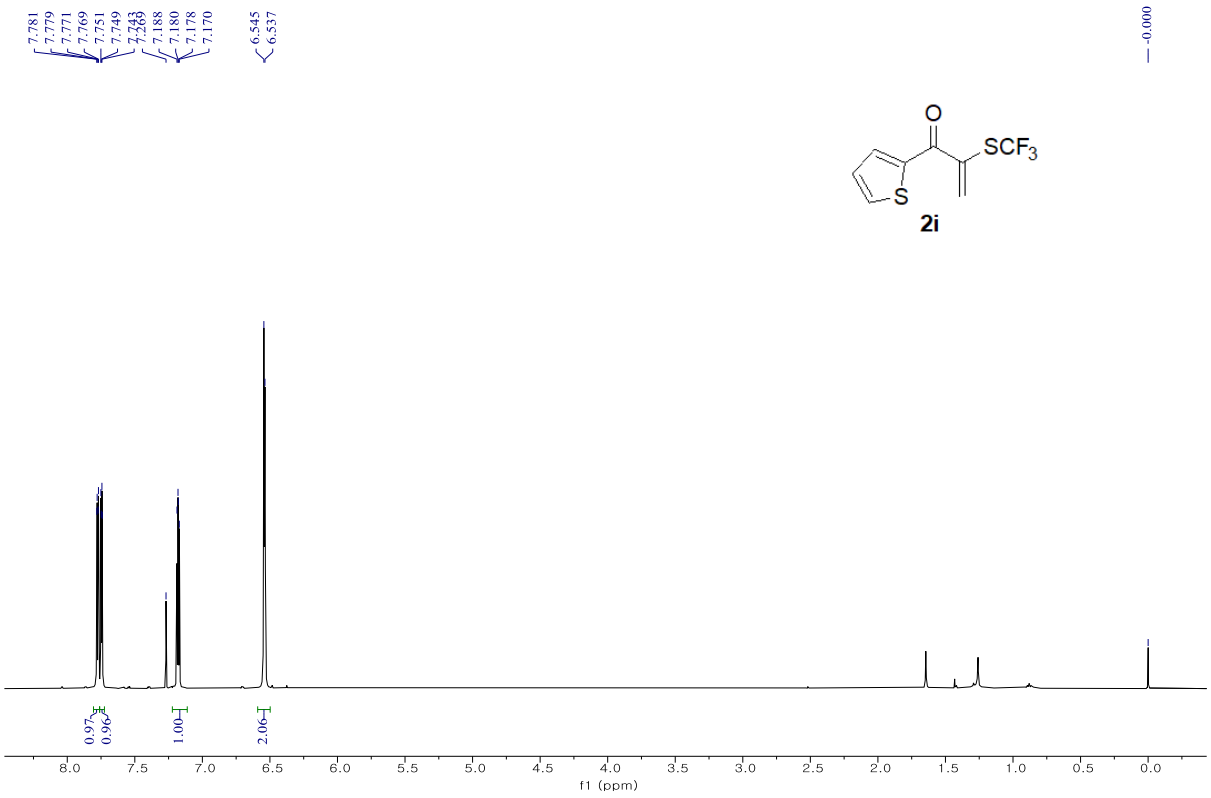

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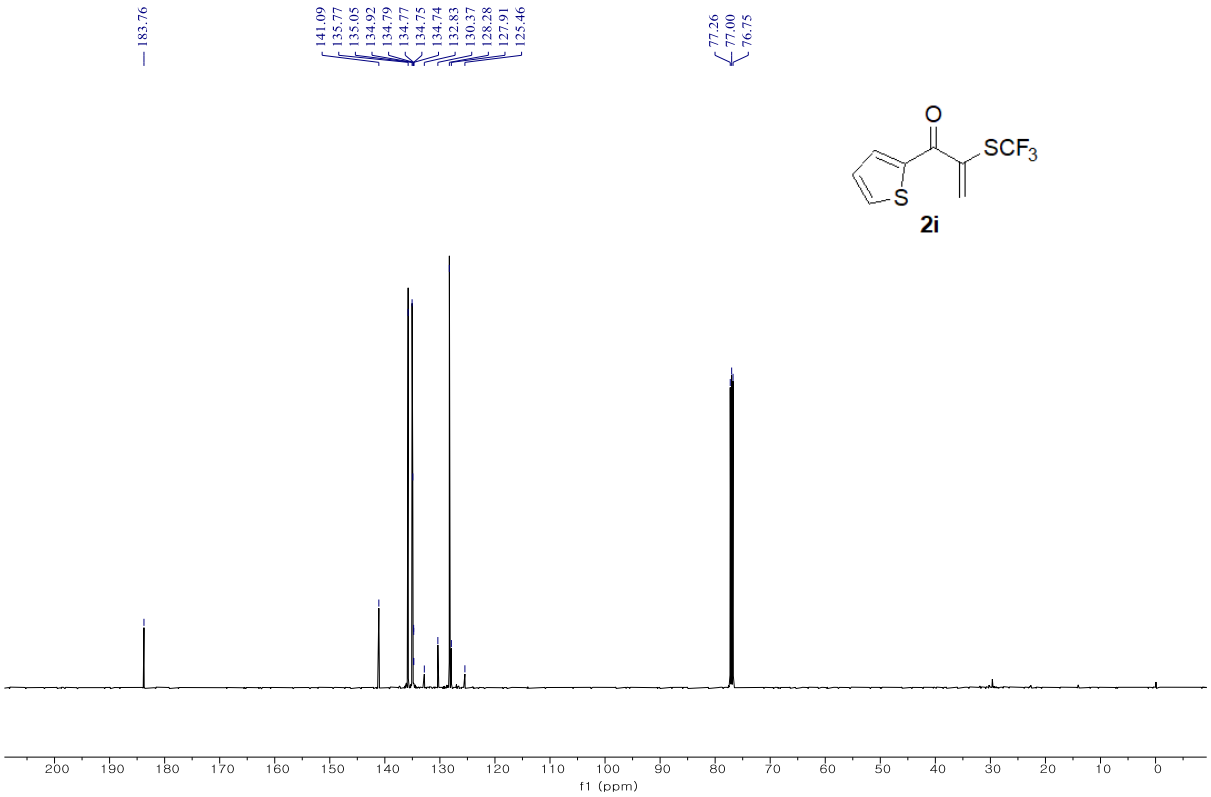
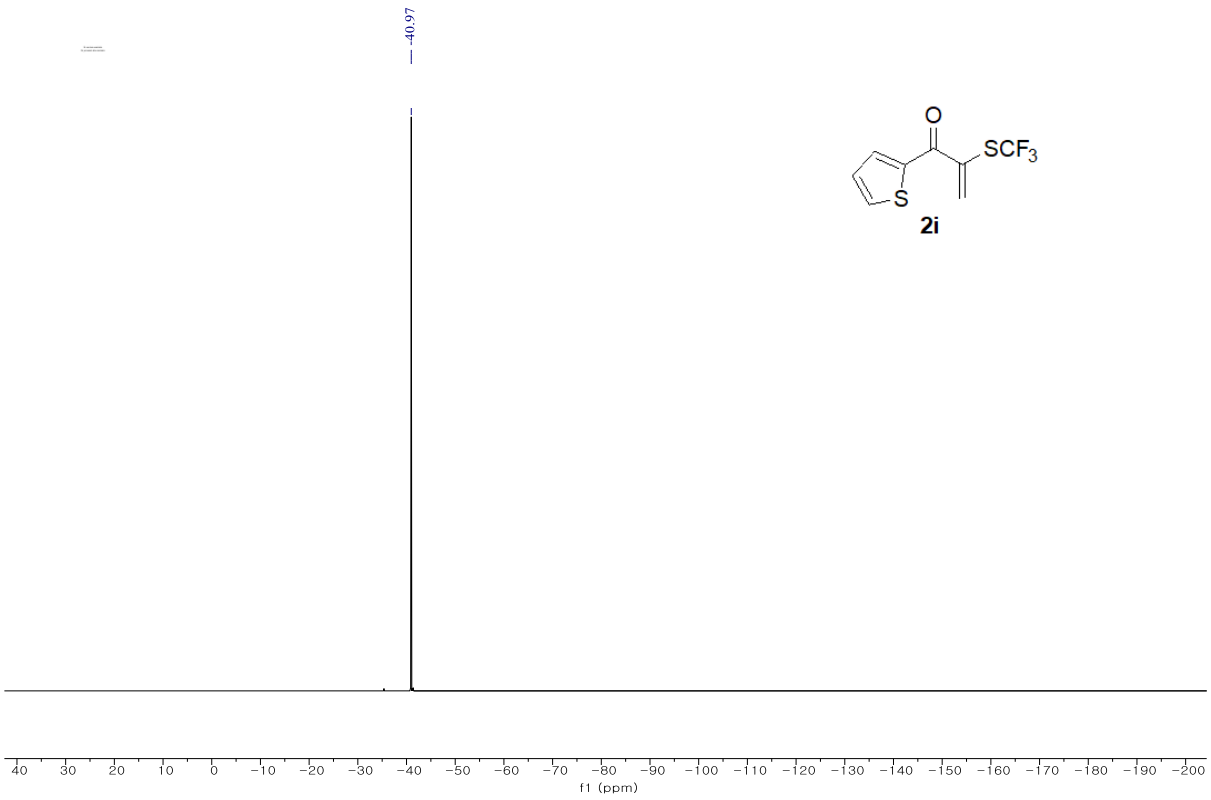


*^{19}F NMR of **2i** (564 MHz, $CDCl_3$)*



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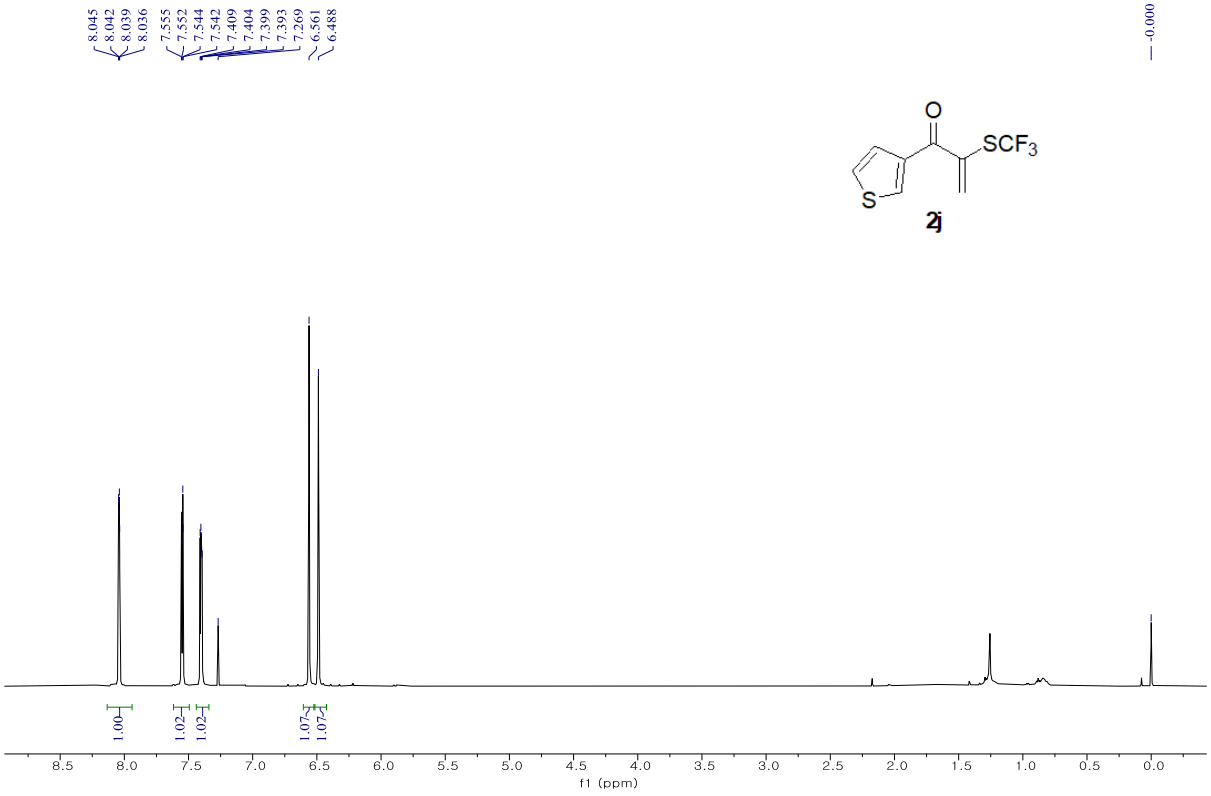
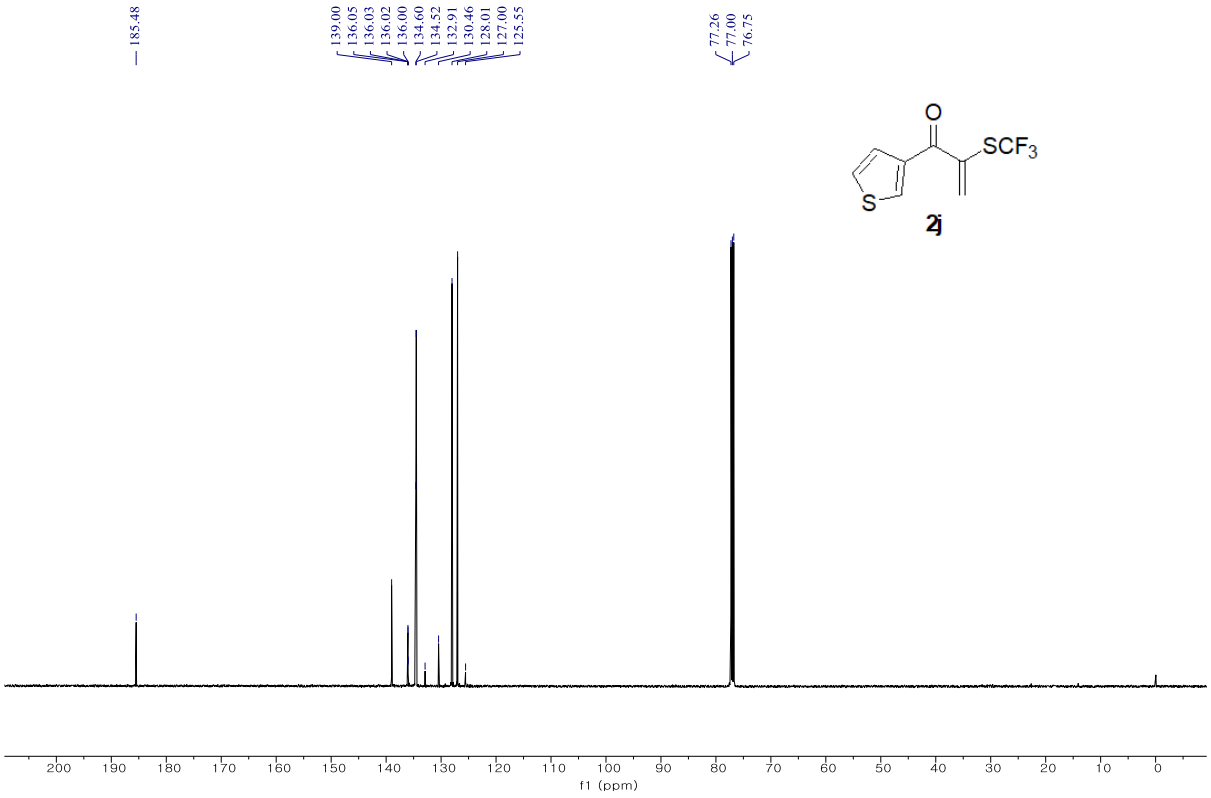


*^{13}C NMR of **2j** (125 MHz, $CDCl_3$)*



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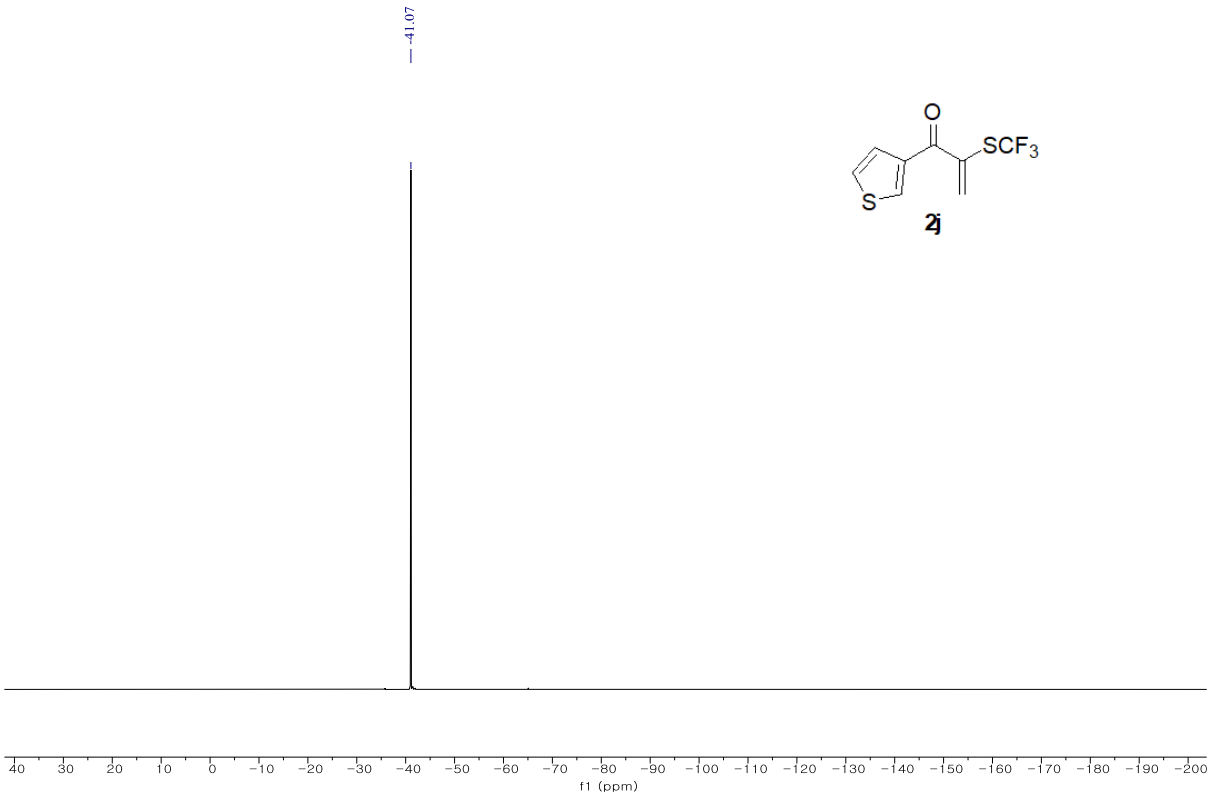
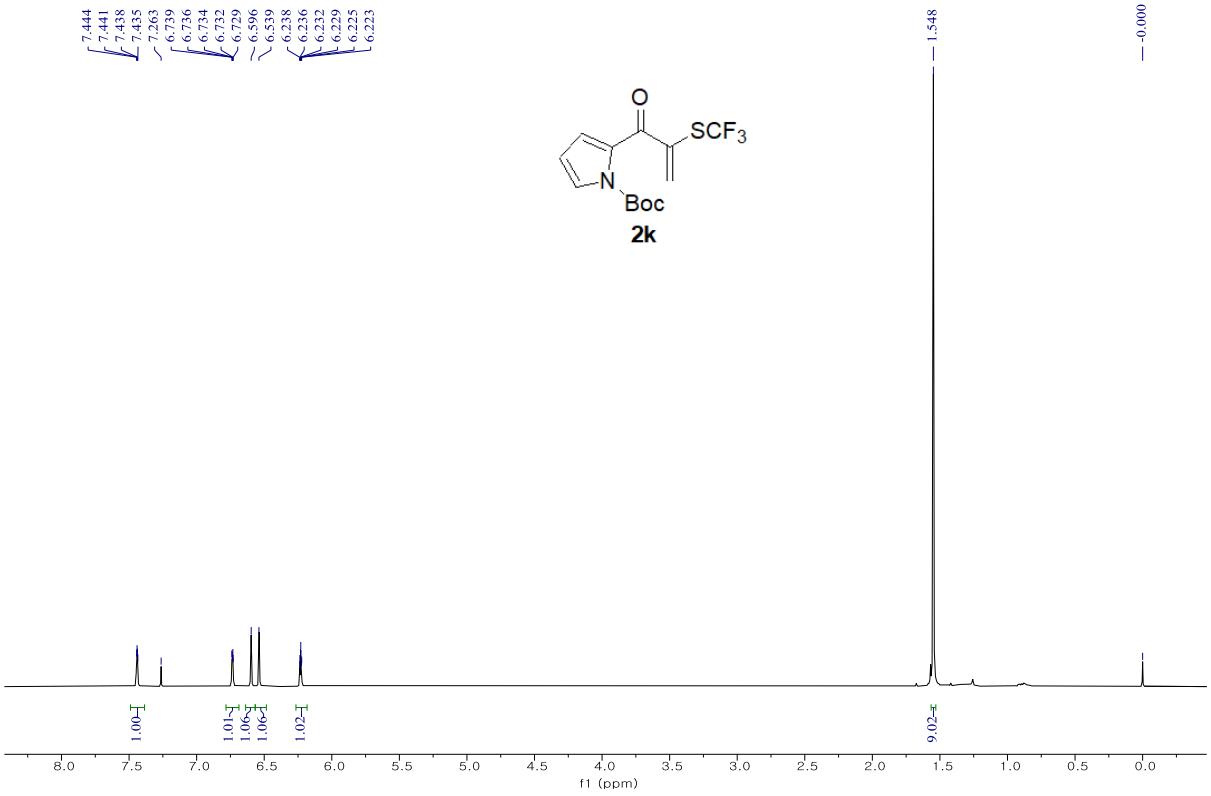
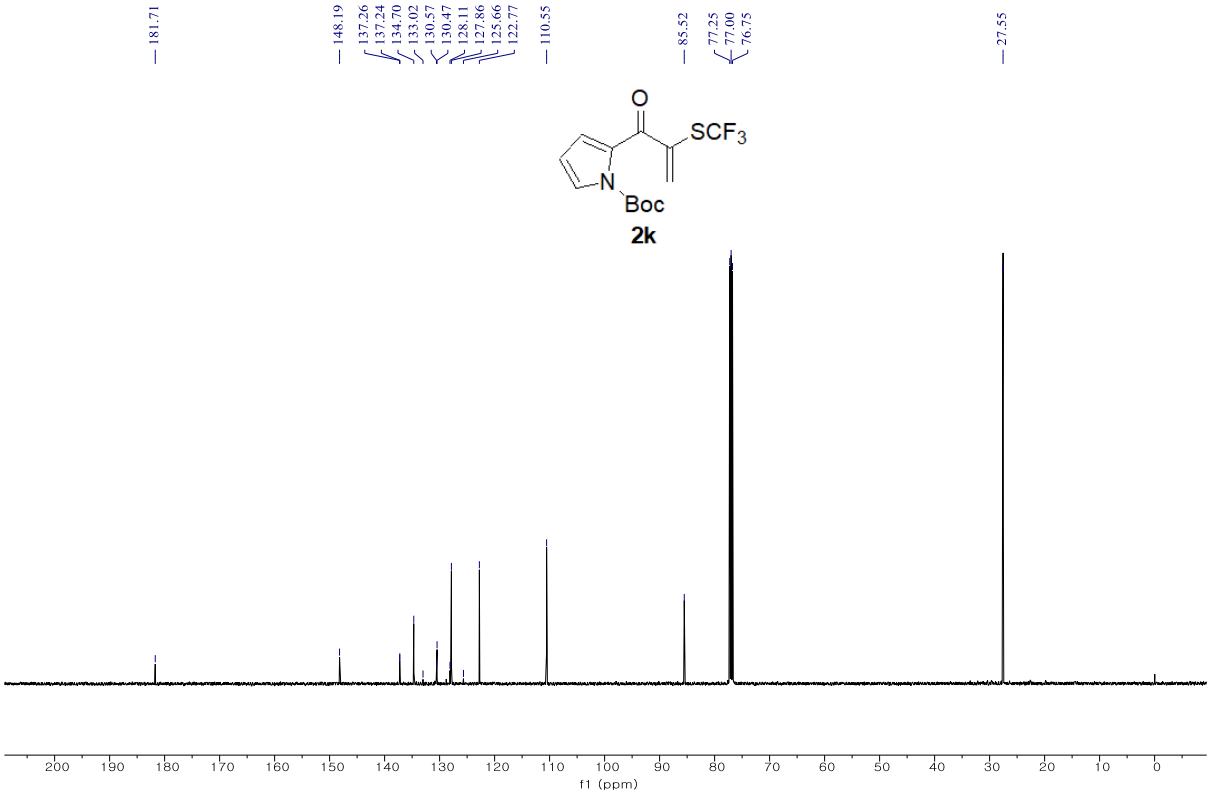


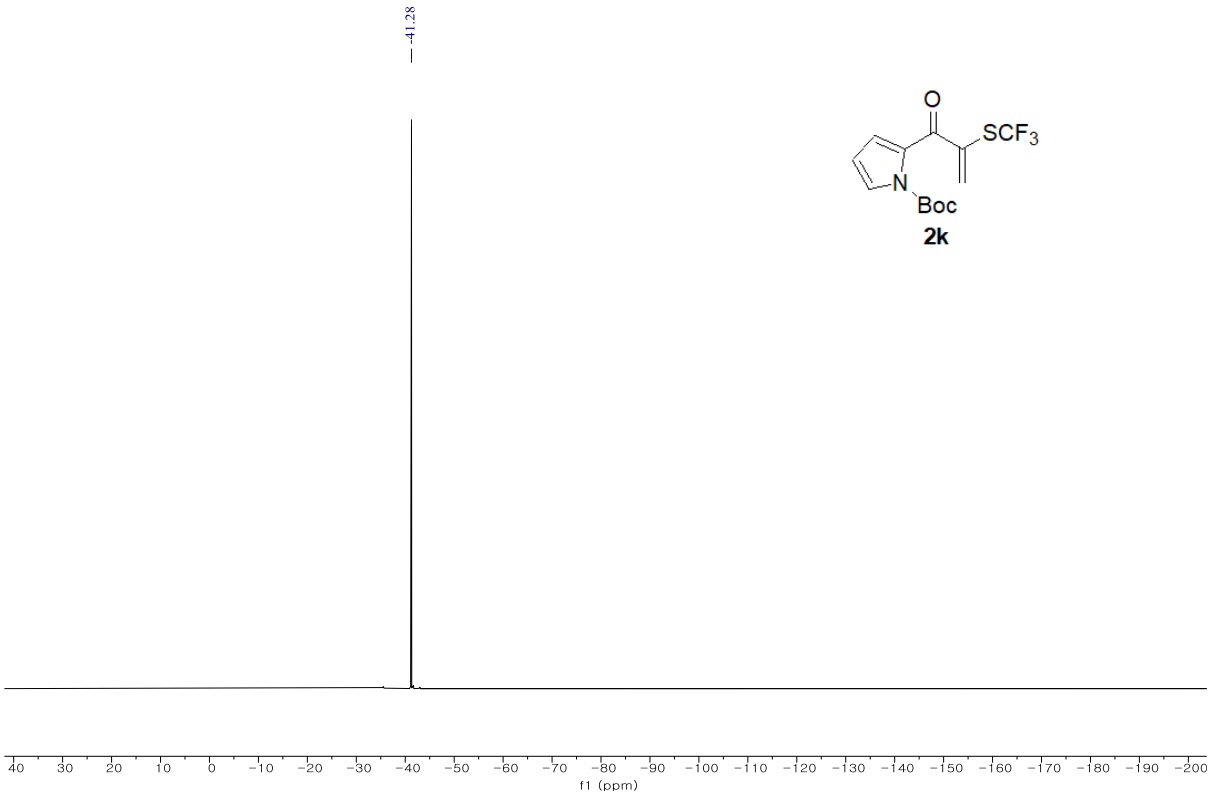
*[1]H NMR of **2k** (500 MHz, $CDCl_3$)*



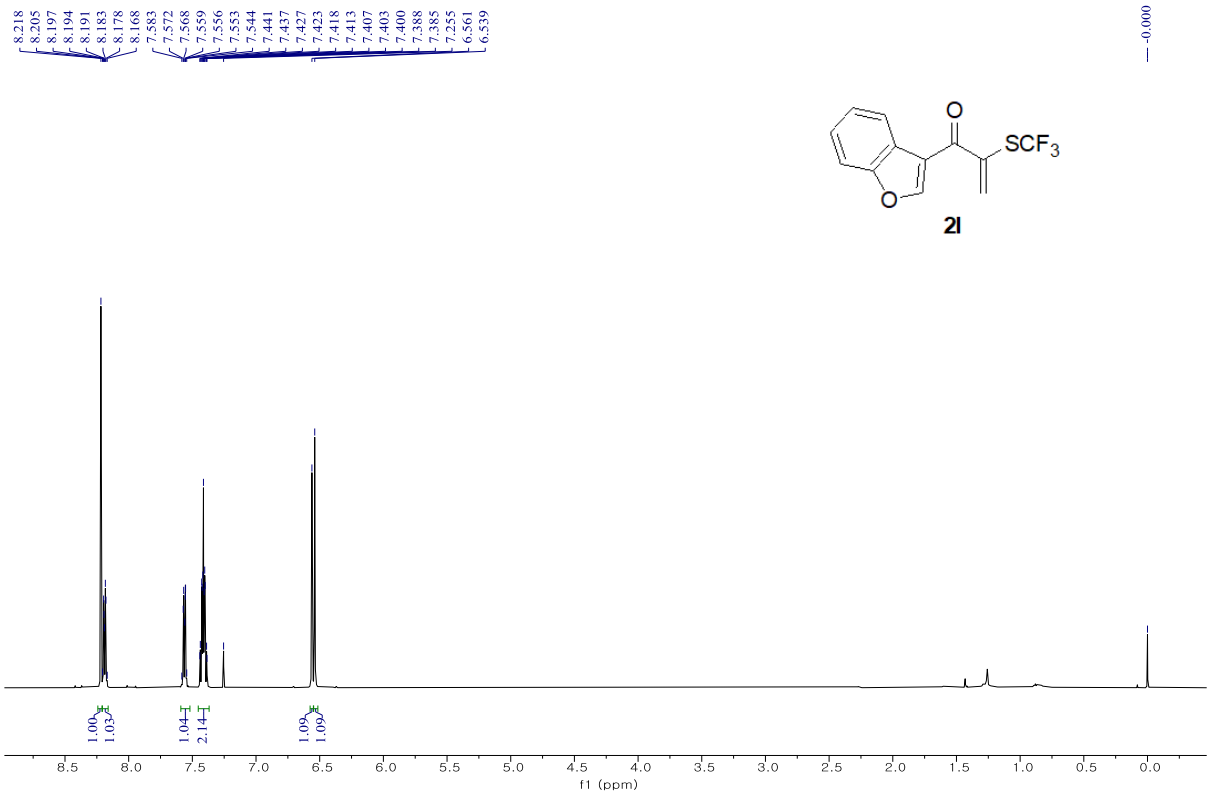
*[13]C NMR of **2k** (125 MHz, $CDCl_3$)*



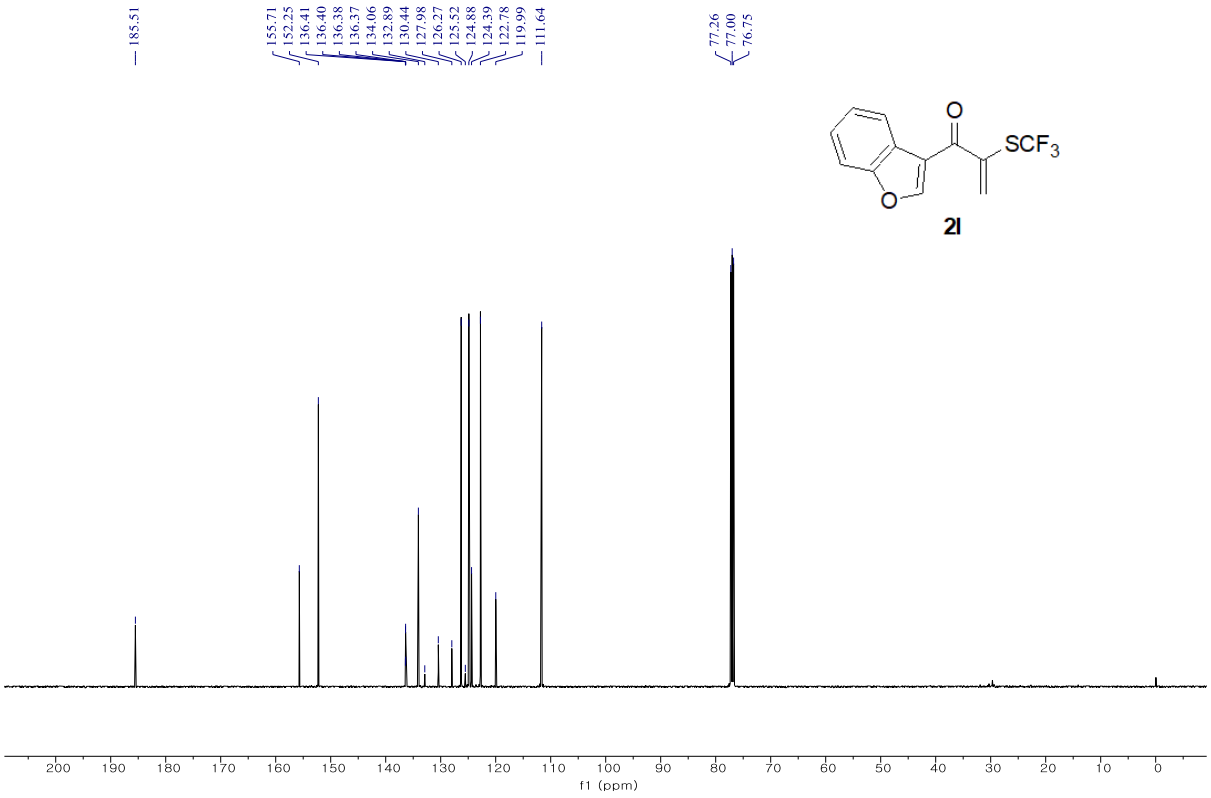
*^{19}F NMR of **2k** (564 MHz, $CDCl_3$)*



*^{1}H NMR of **2l** (500 MHz, $CDCl_3$)*



*^{13}C NMR of **2l** (125 MHz, $CDCl_3$)*



*^{19}F NMR of **2l** (564 MHz, $CDCl_3$)*

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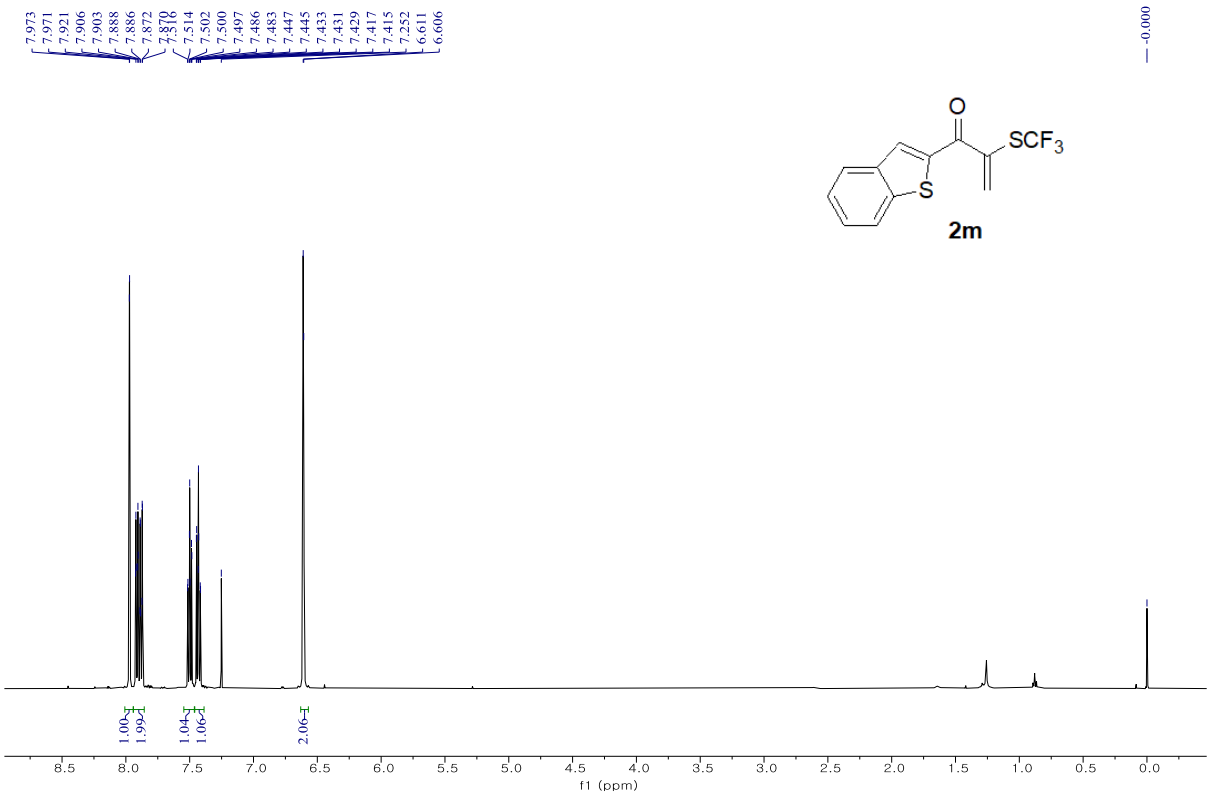

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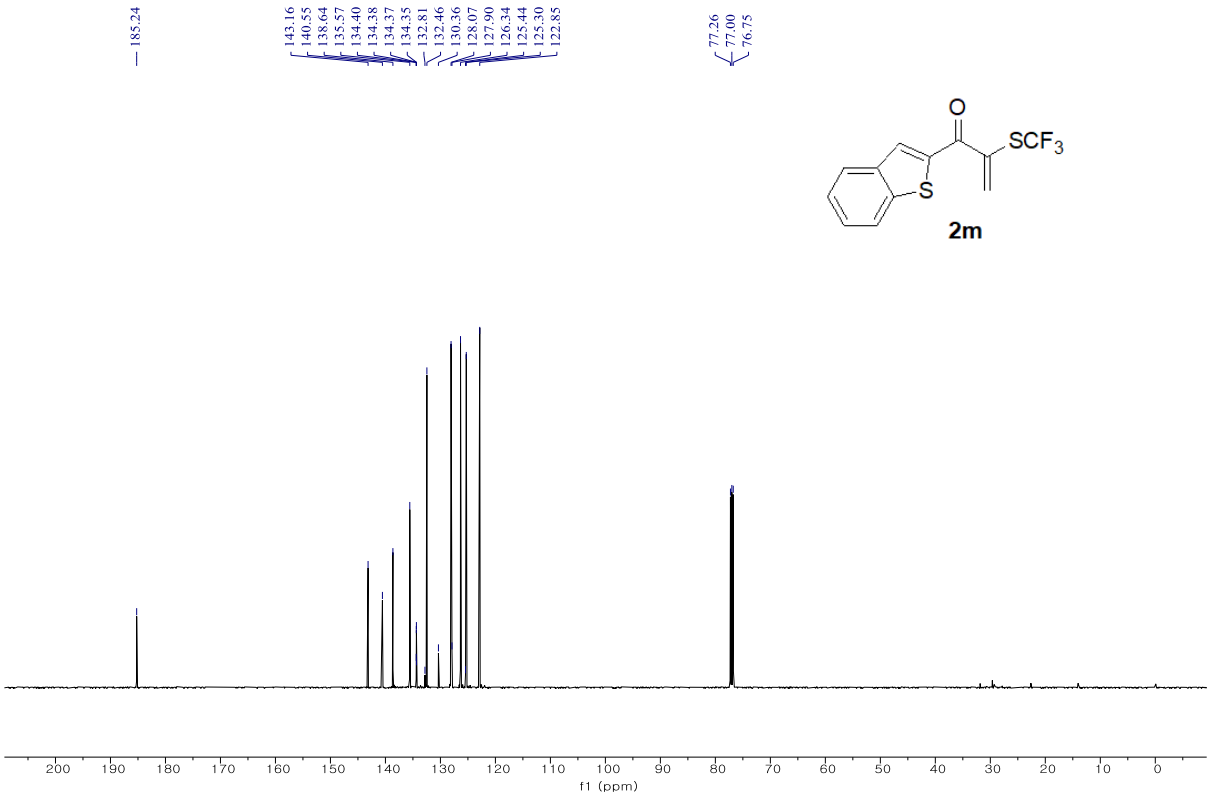
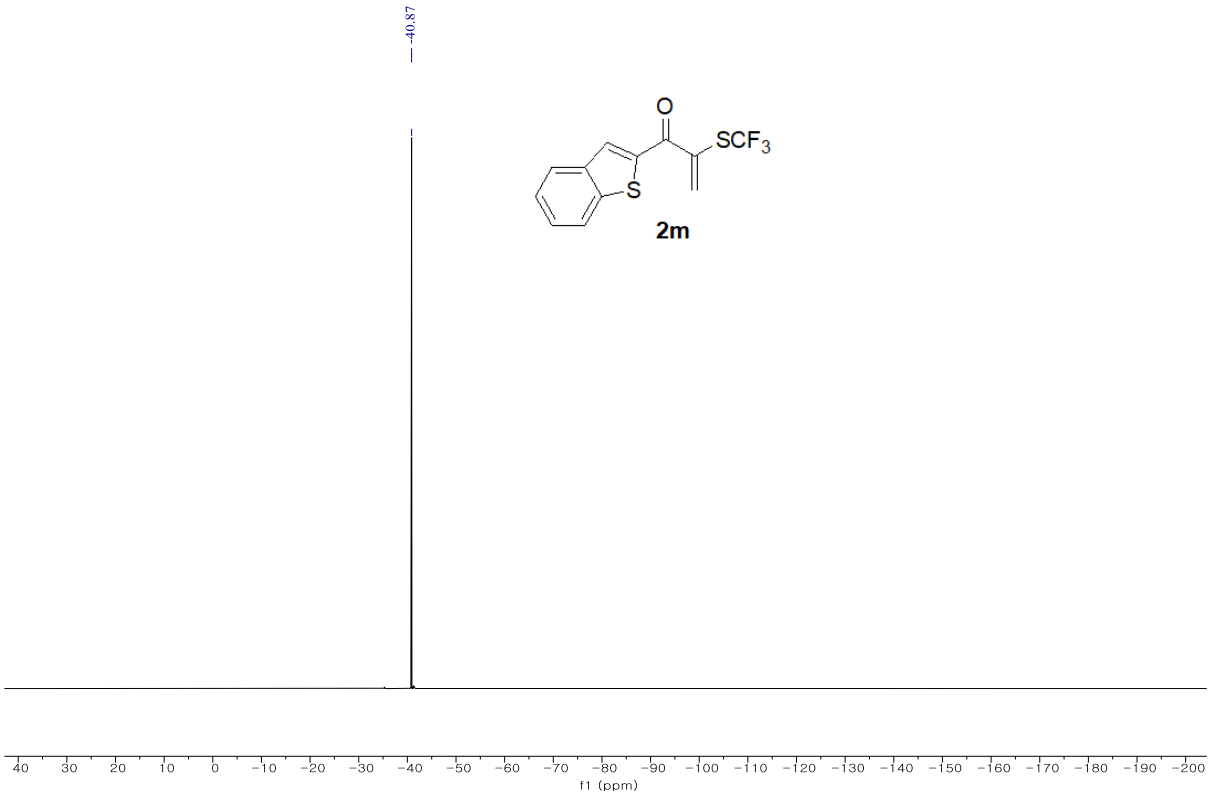
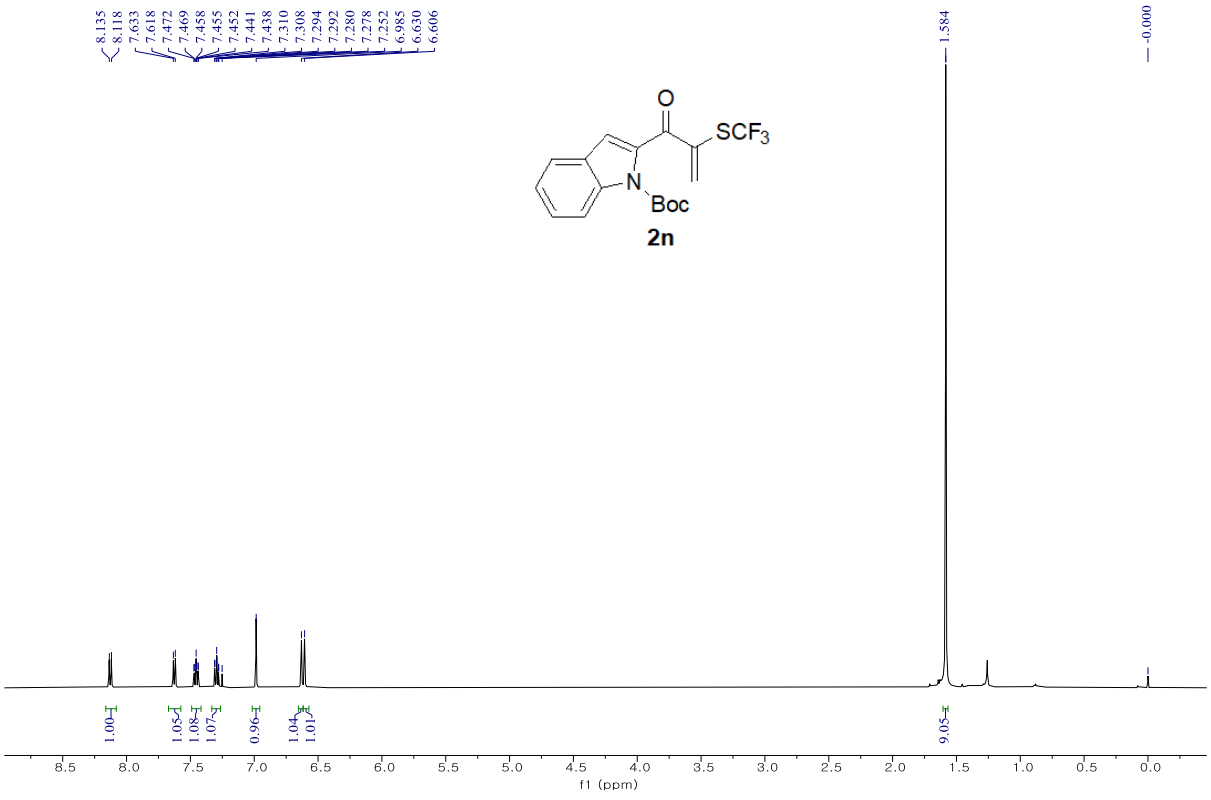


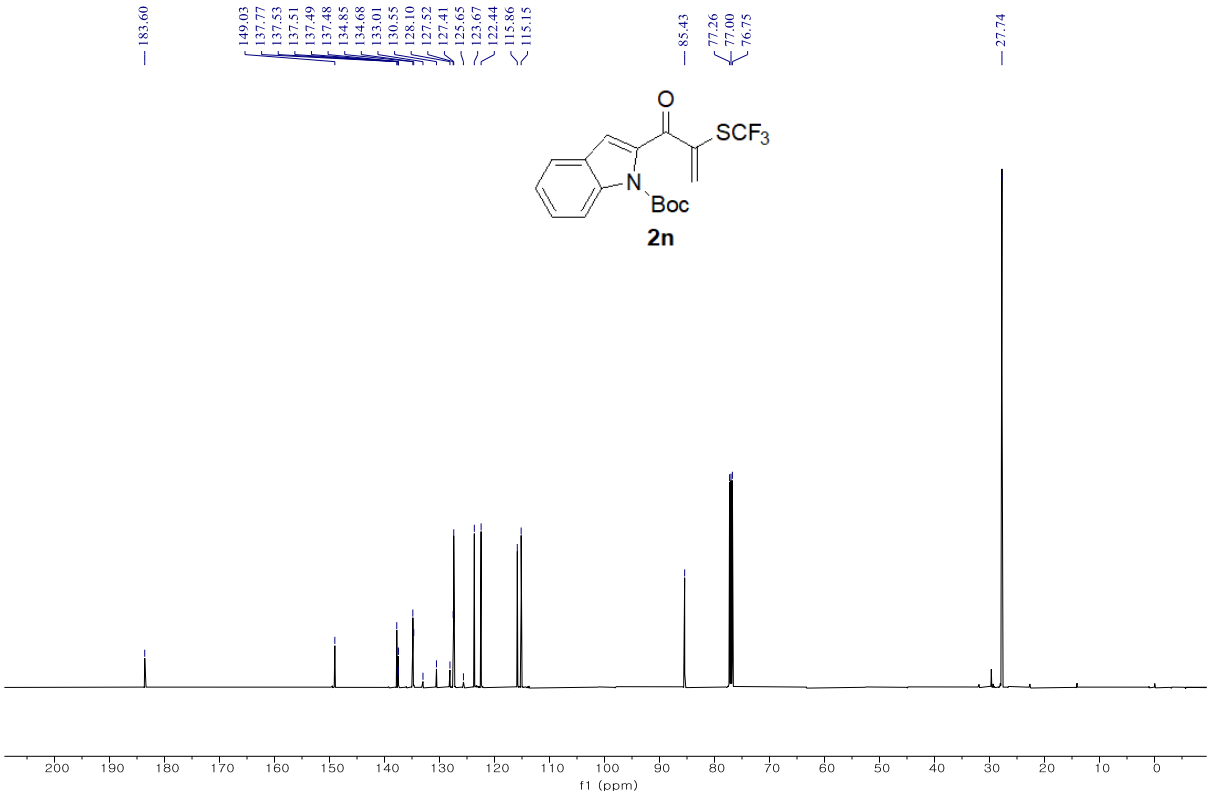
*^{19}F NMR of **2m** (564 MHz, $CDCl_3$)*



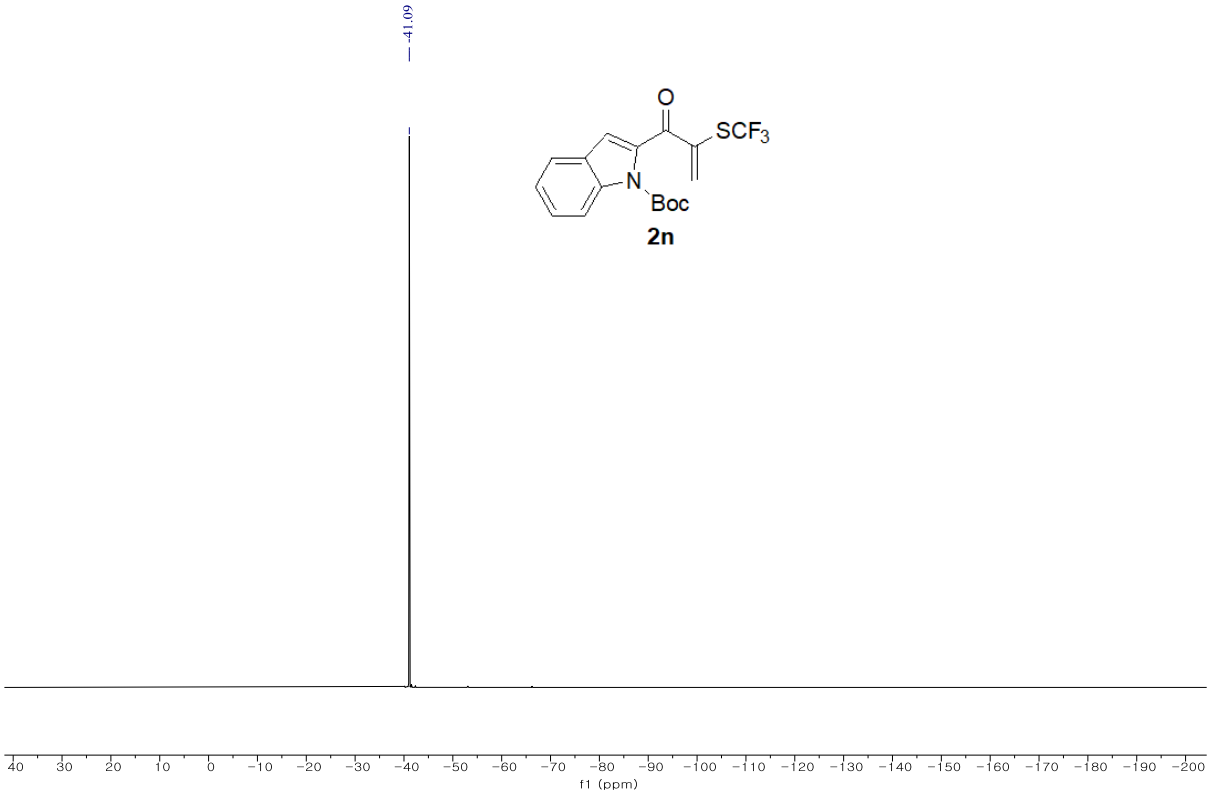
*^{1}H NMR of **2n** (500 MHz, $CDCl_3$)*



*^{13}C NMR of **2n** (125 MHz, $CDCl_3$)*



*^{19}F NMR of **2n** (564 MHz, $CDCl_3$)*



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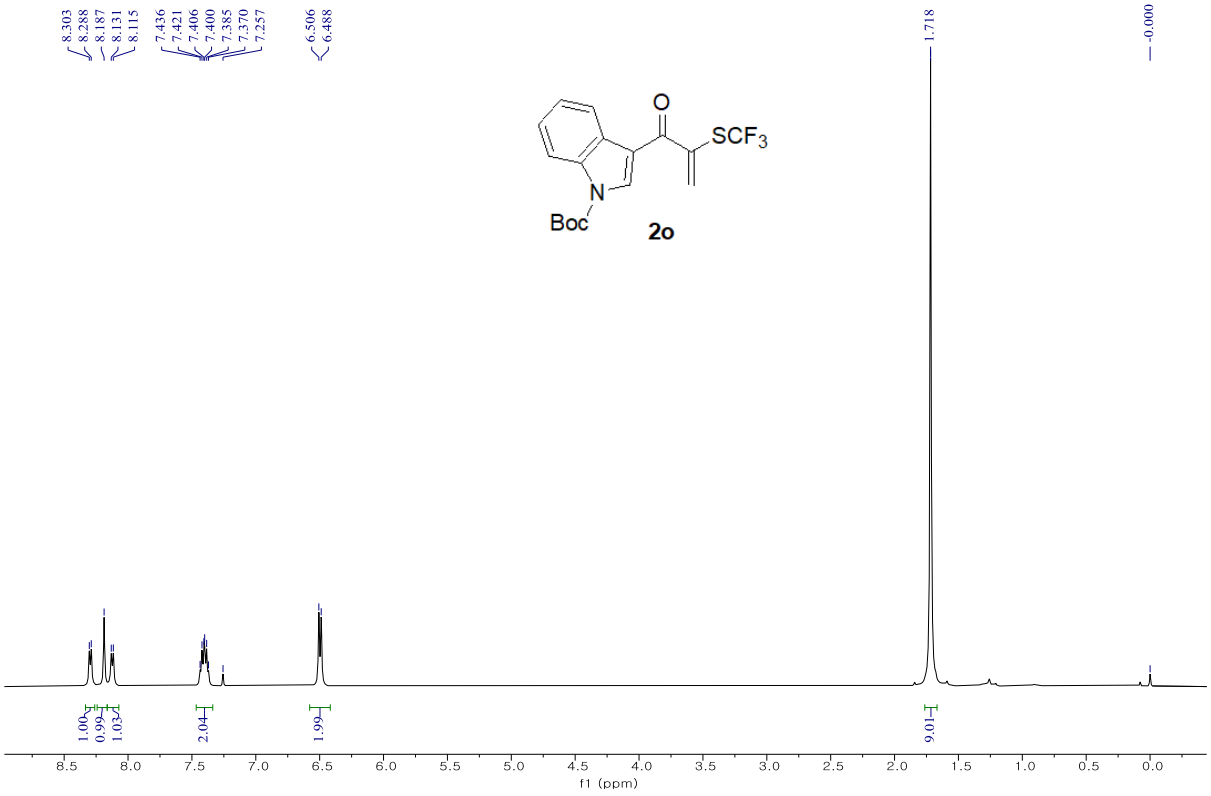

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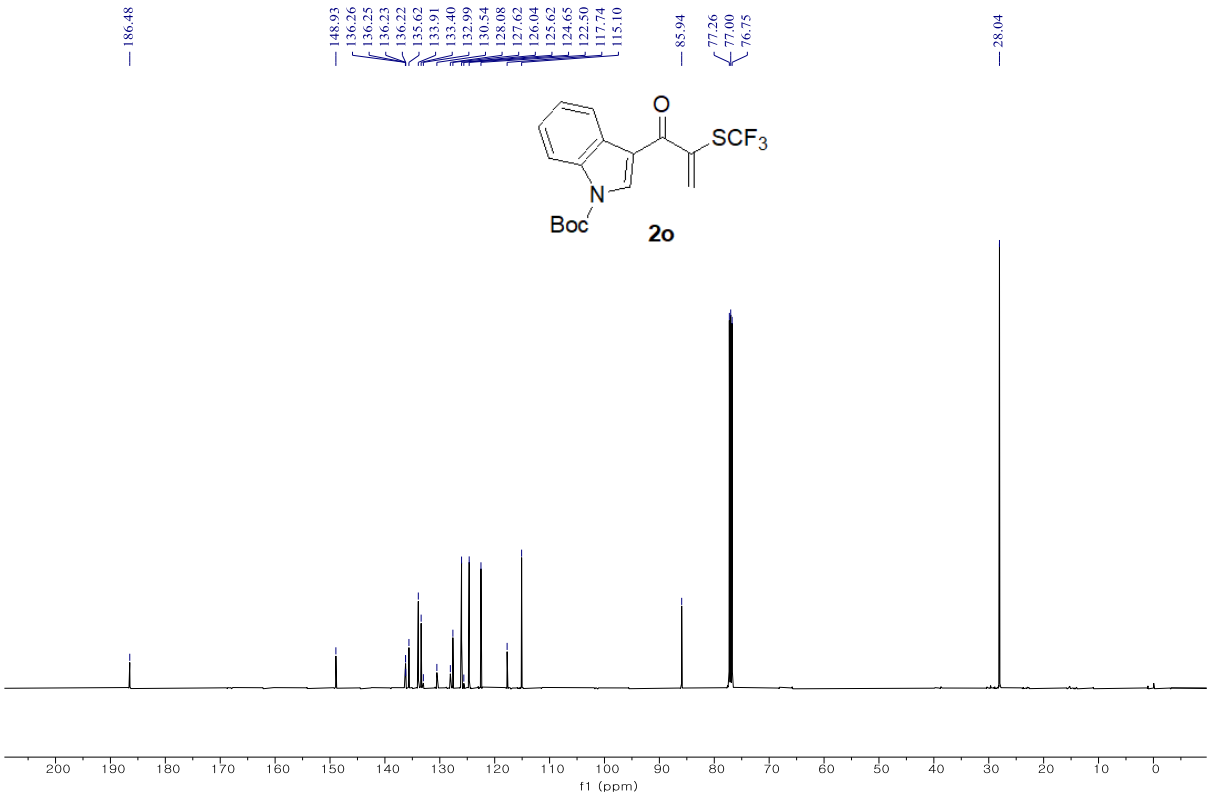
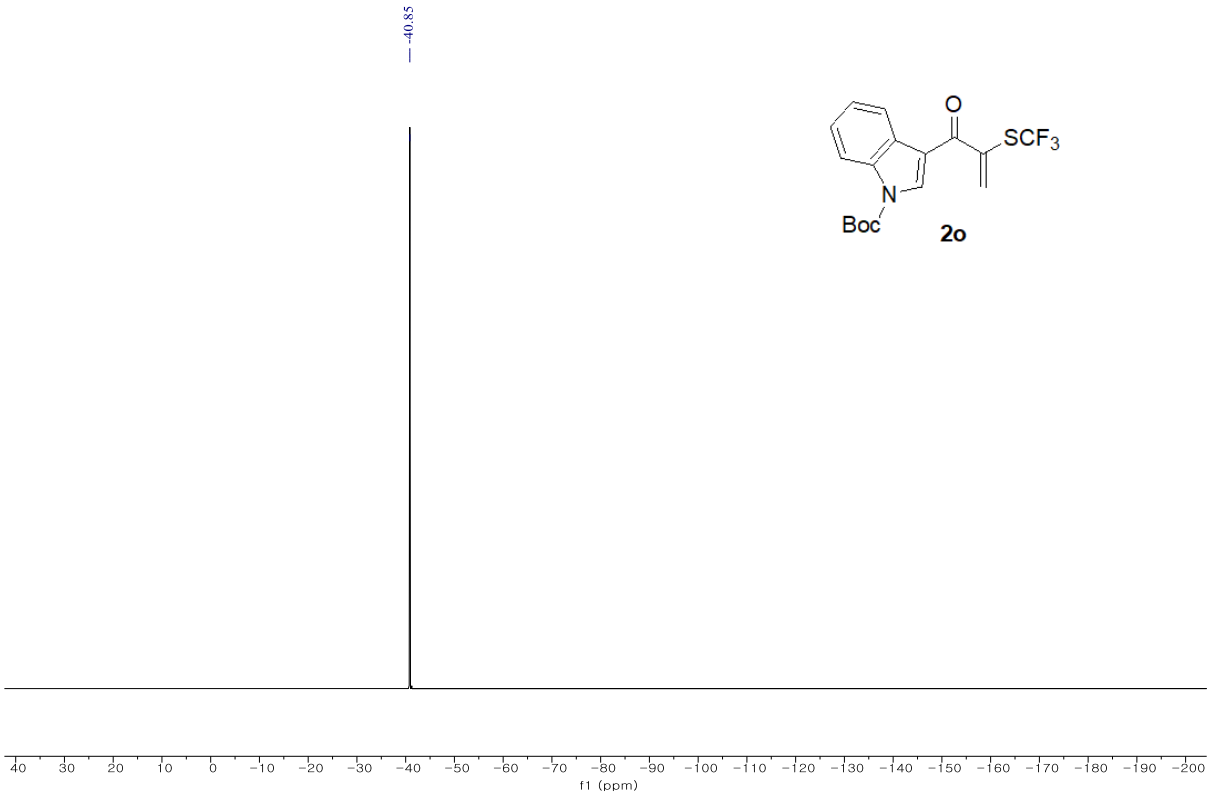


*^{19}F NMR of **2o** (564 MHz, $CDCl_3$)*



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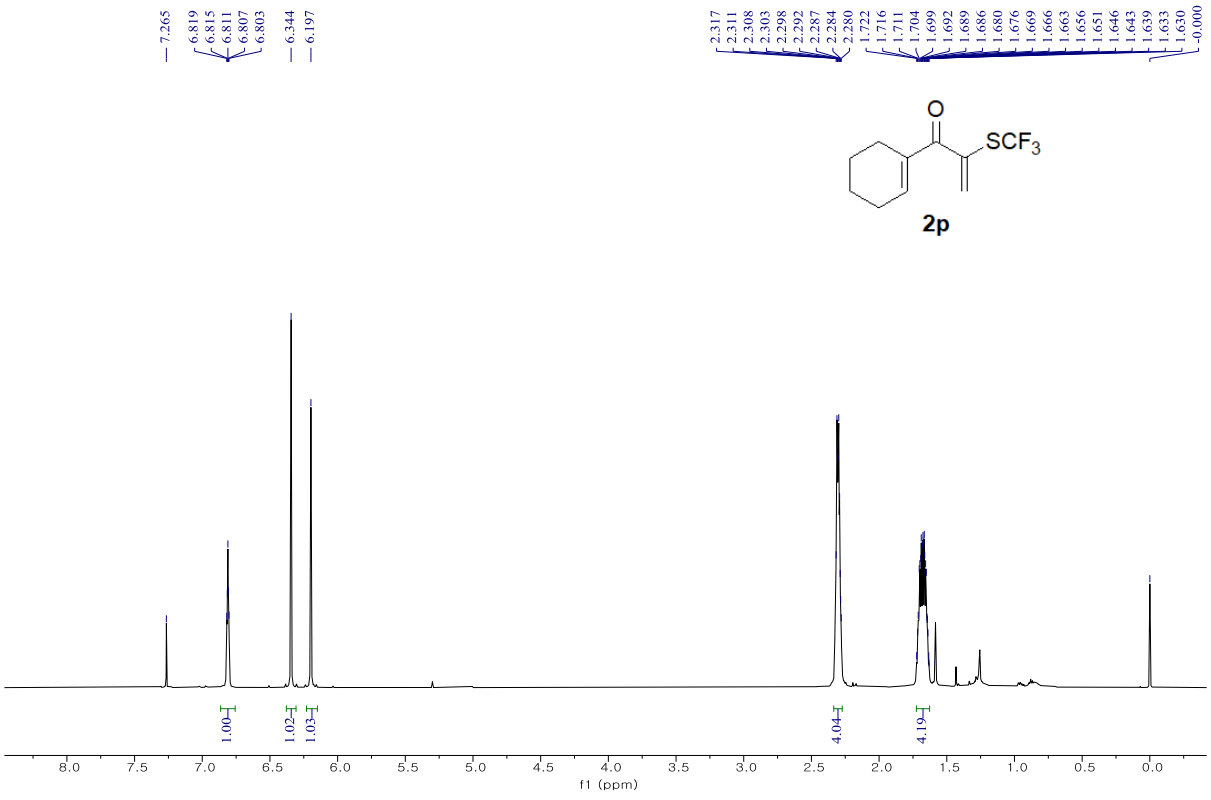
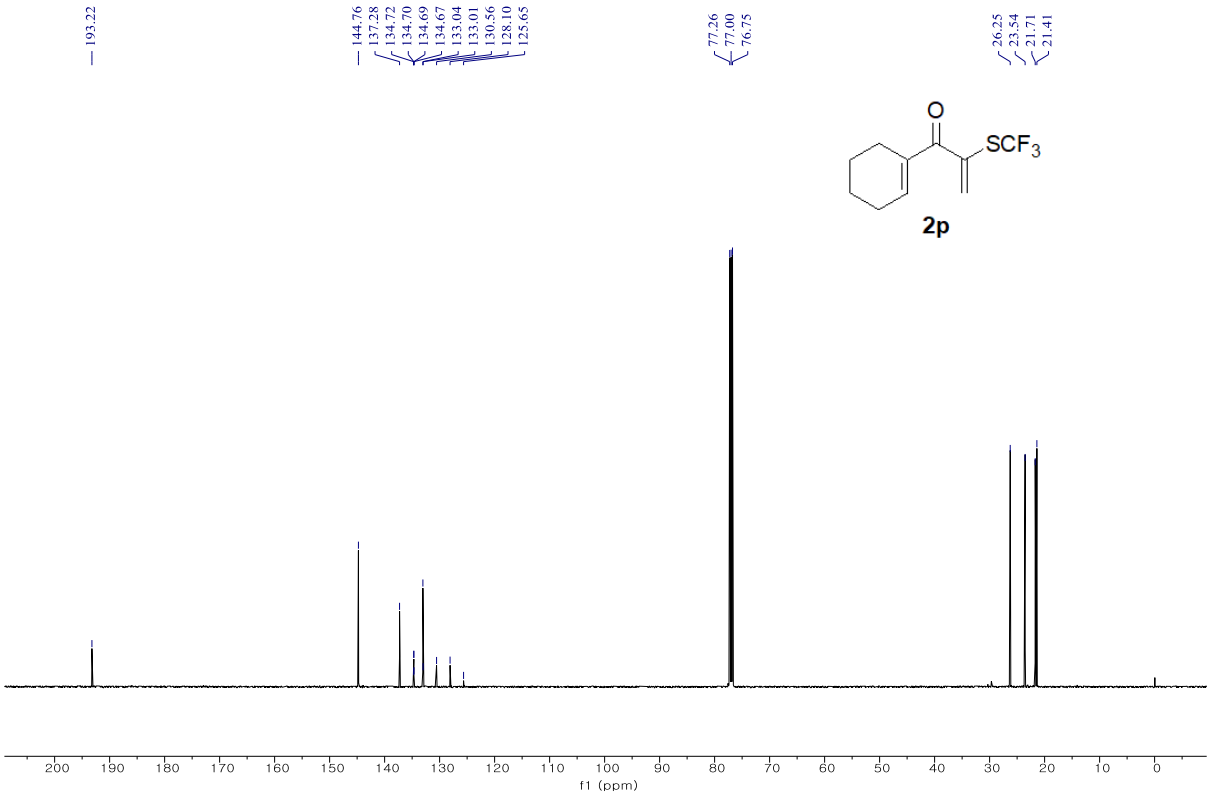
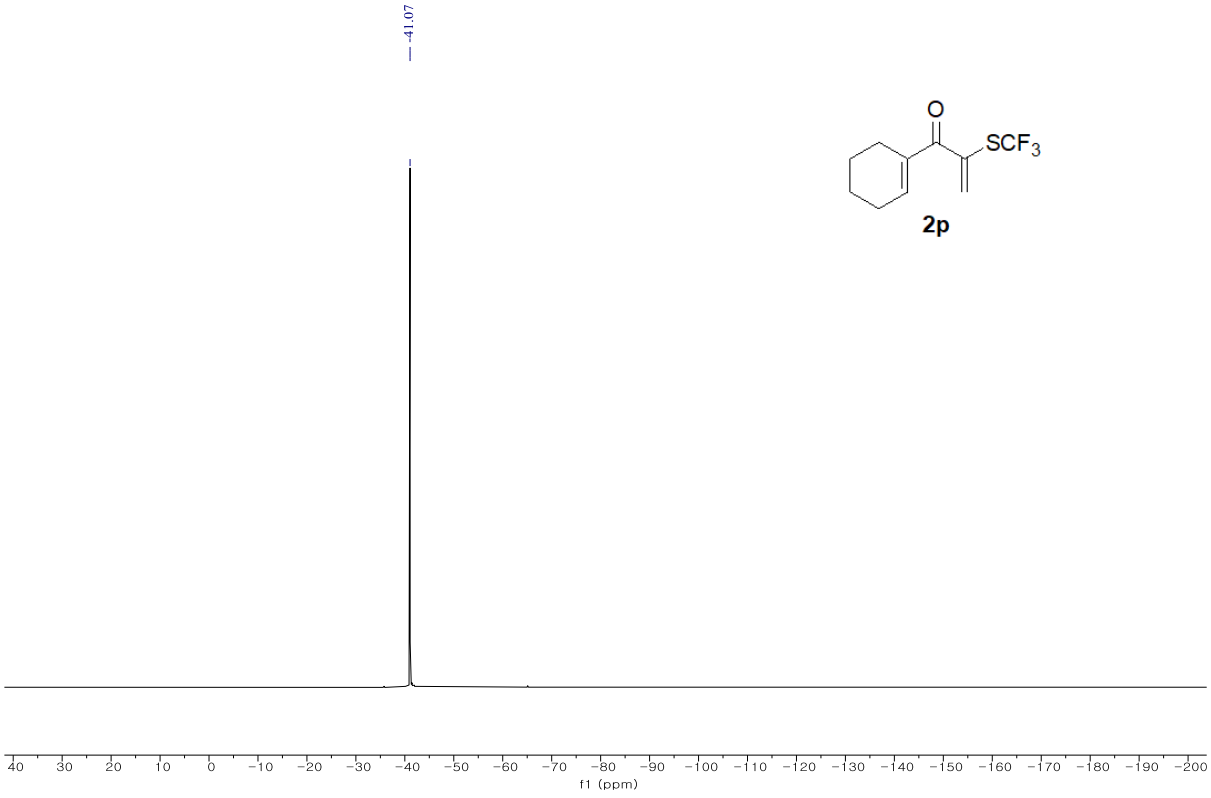


*^{13}C NMR of **2p** (125 MHz, $CDCl_3$)*



*^{19}F NMR of **2p** (564 MHz, $CDCl_3$)*



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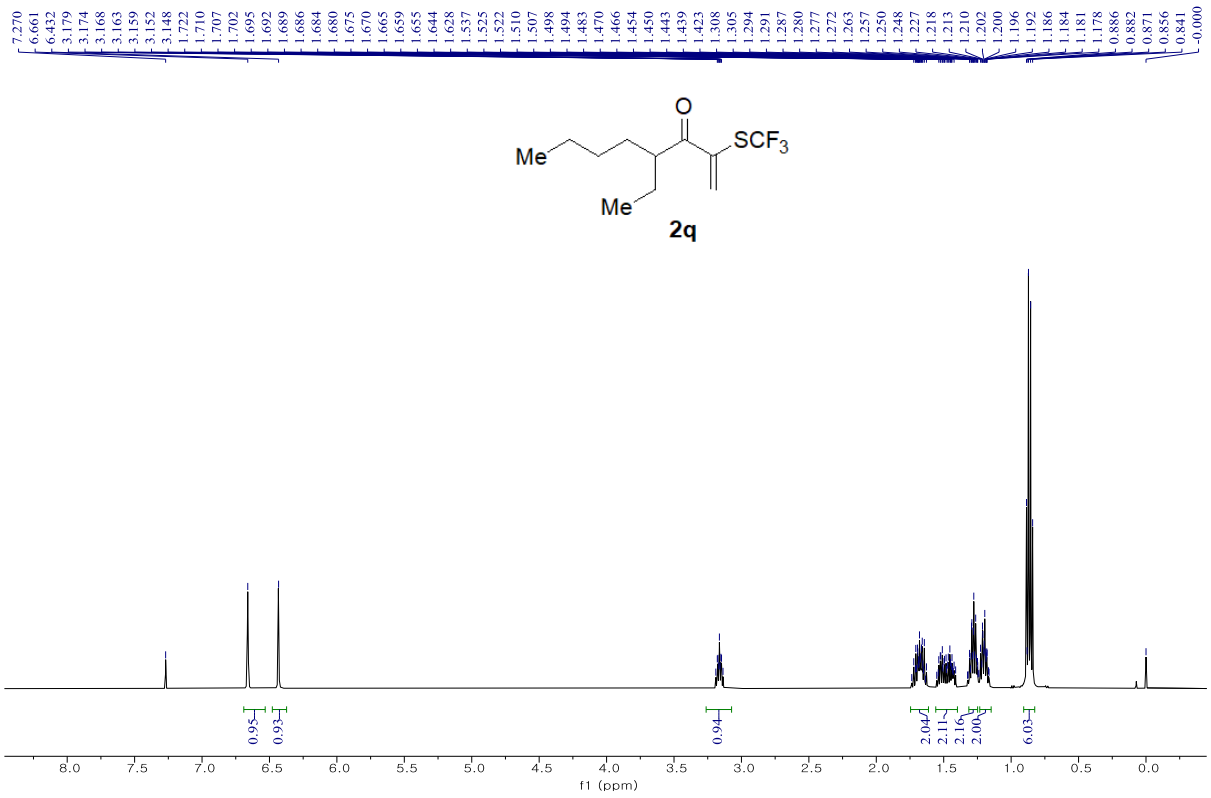
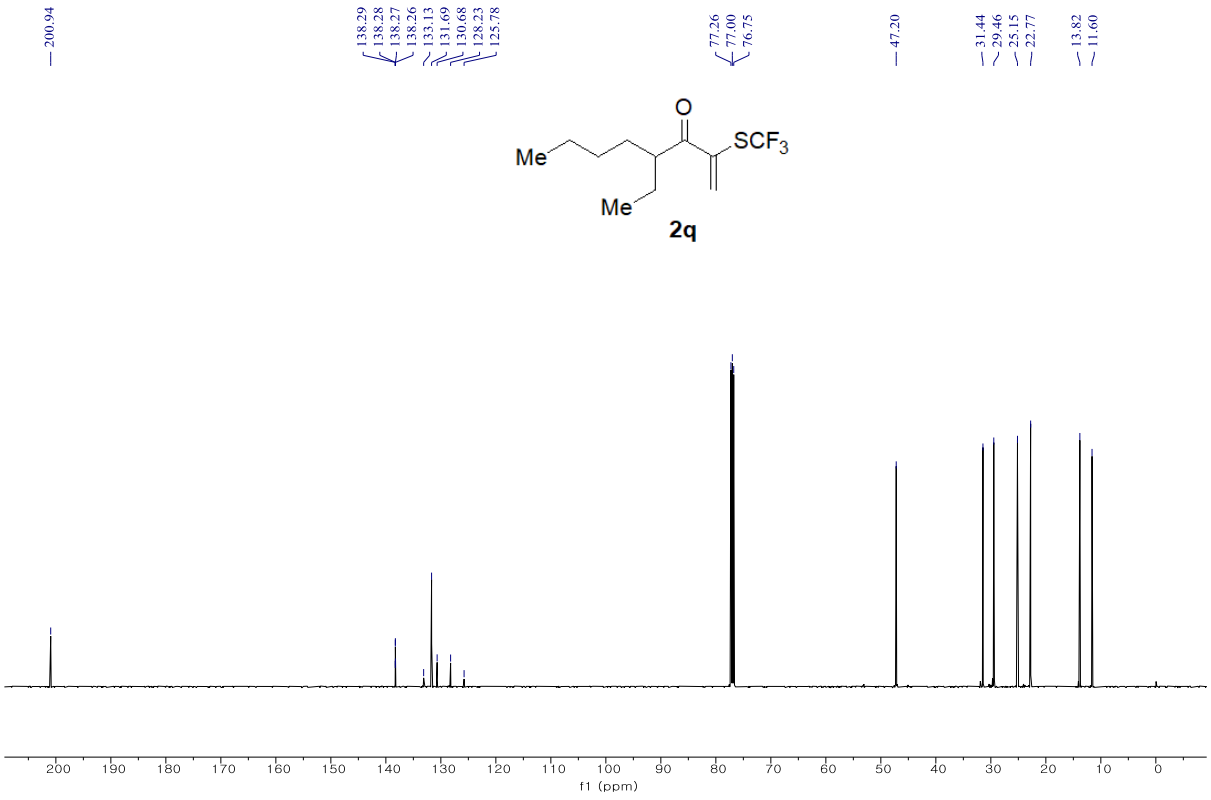
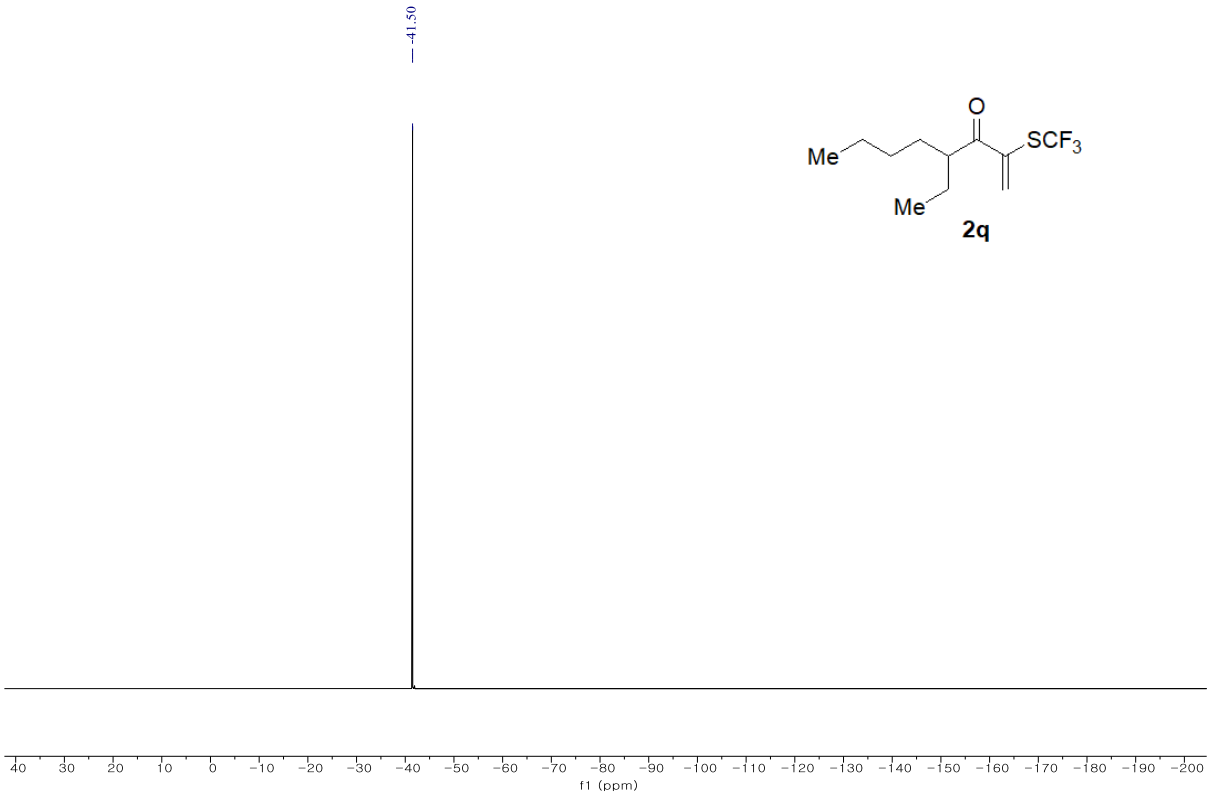


*[13]C NMR of **2q** (125 MHz, CDCl3)*



*^{19}F NMR of **2q** (564 MHz, $CDCl_3$)*



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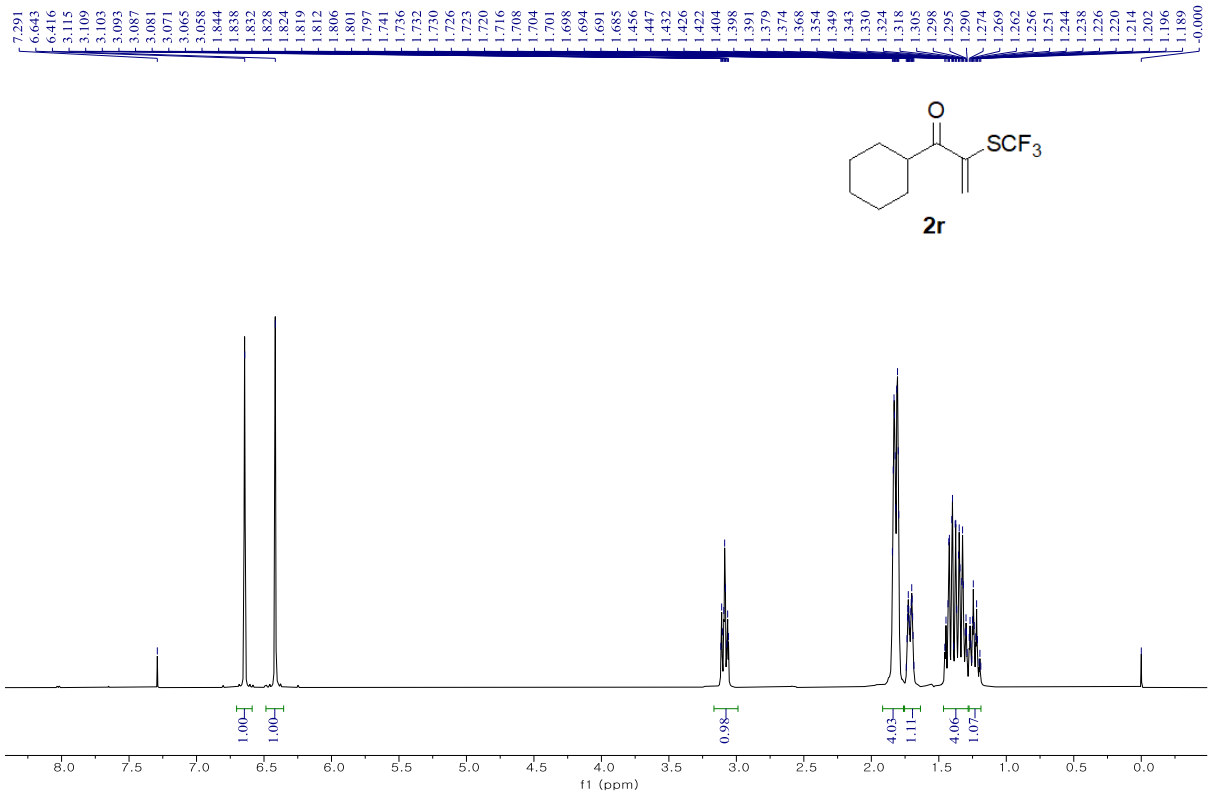
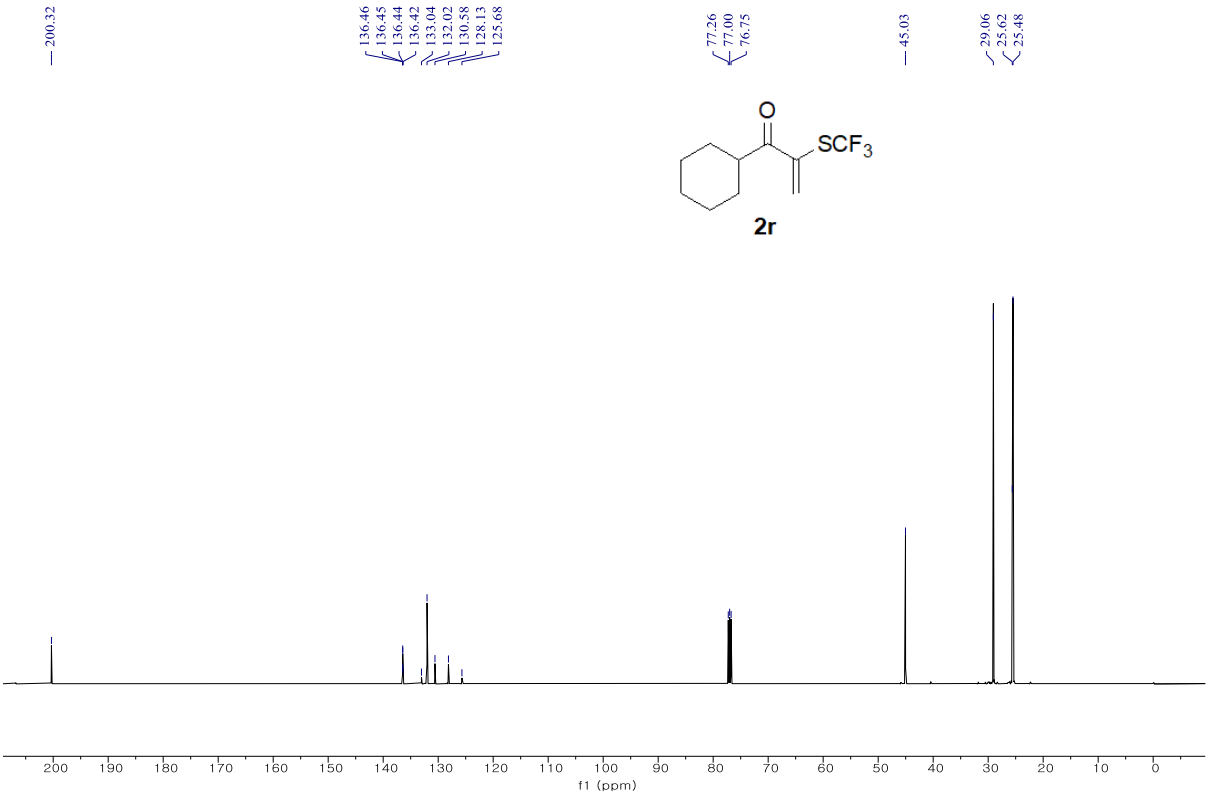
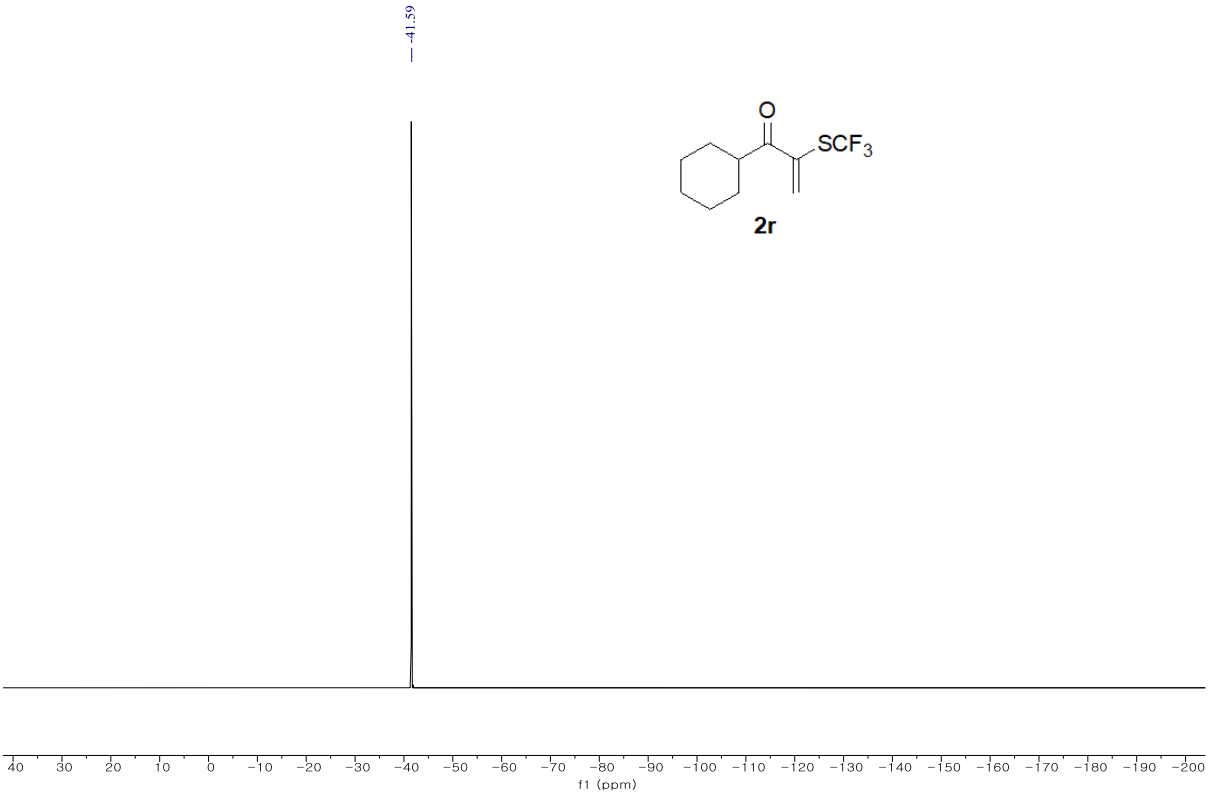


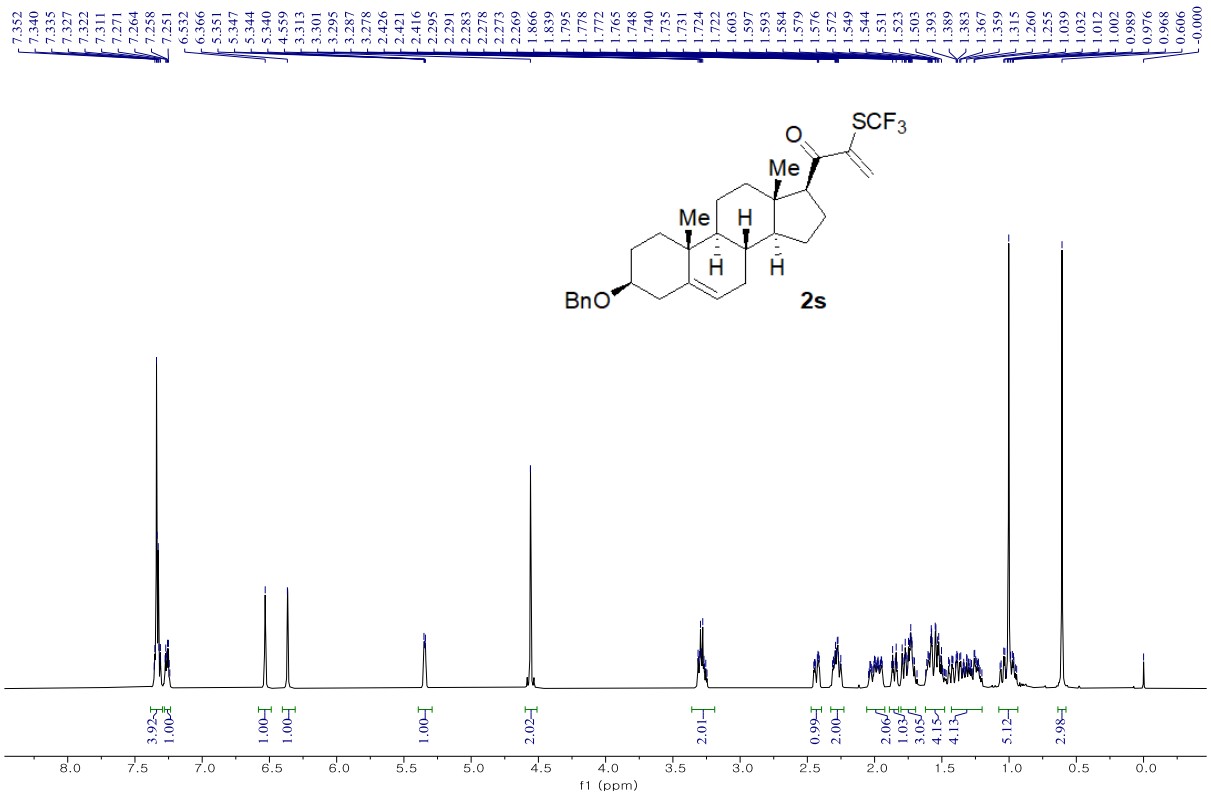
*^{13}C NMR of **2r** (125 MHz, $CDCl_3$)*



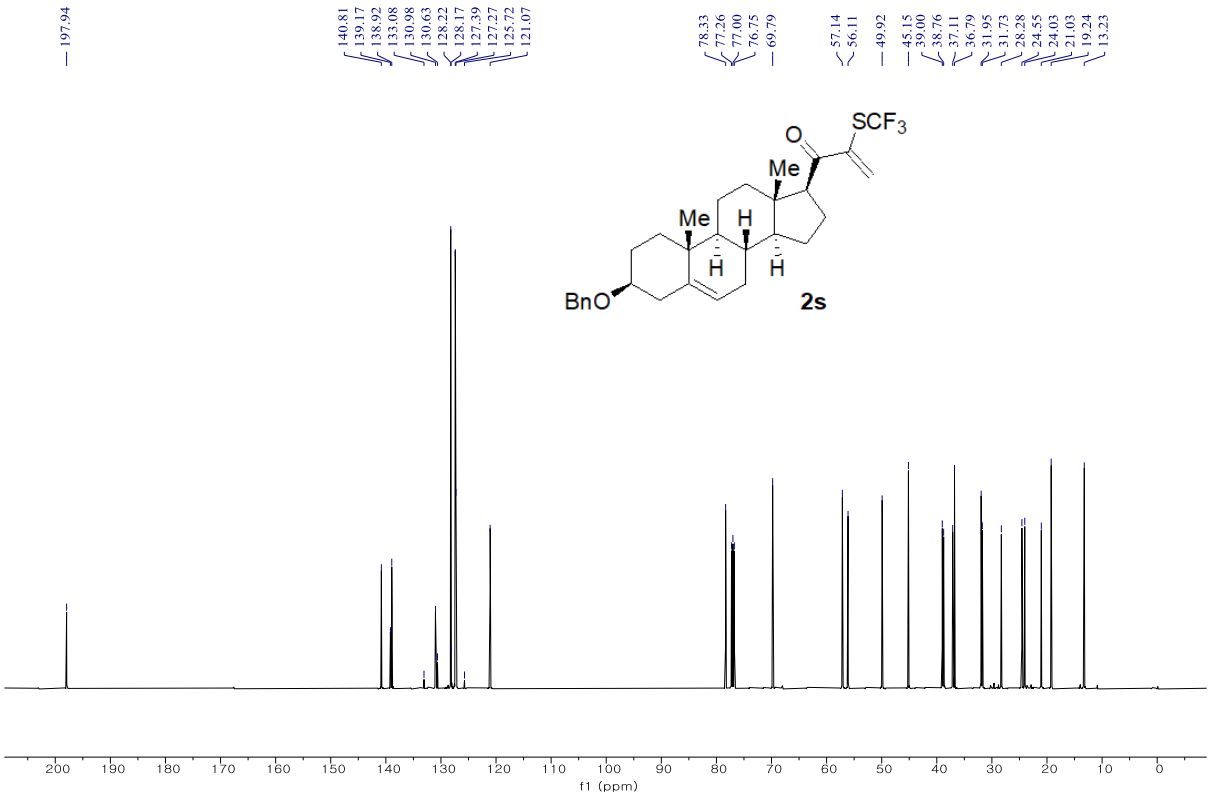
*^{19}F NMR of **2r** (564 MHz, $CDCl_3$)*



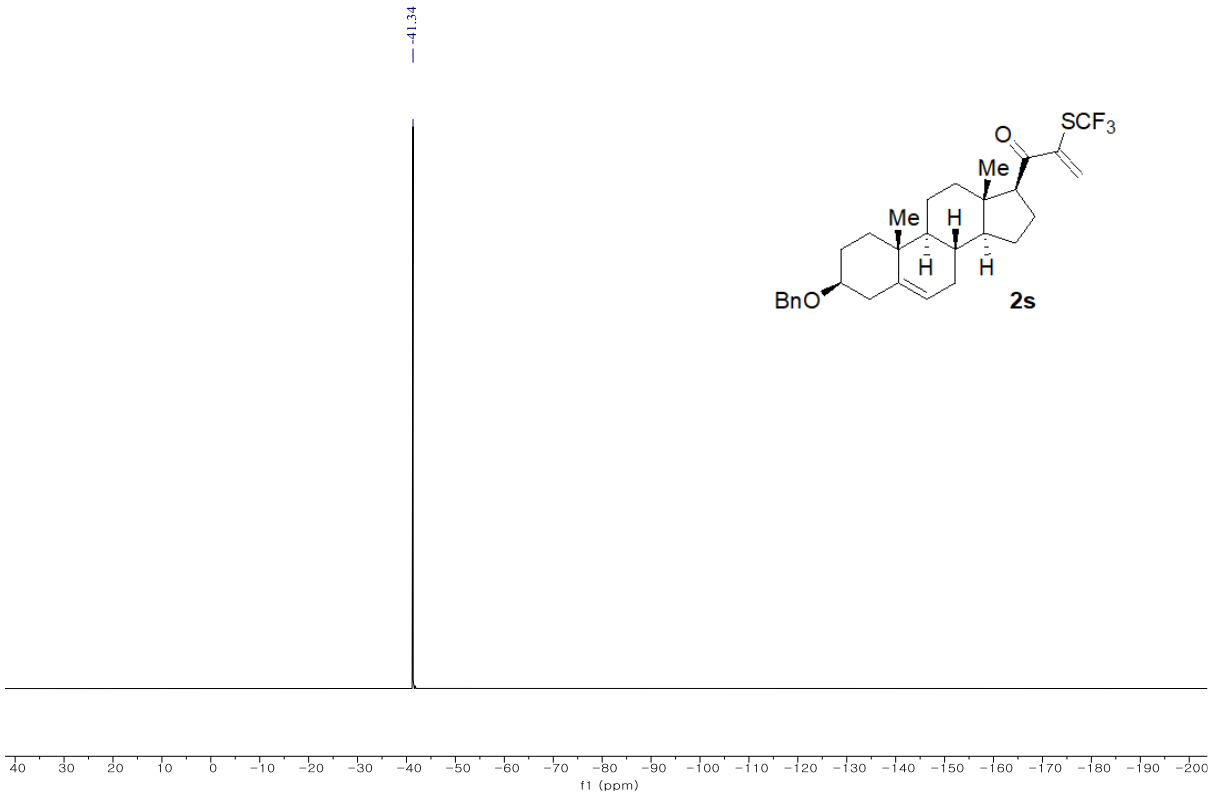
*[1]H NMR of **2s** (500 MHz, $CDCl_3$)*



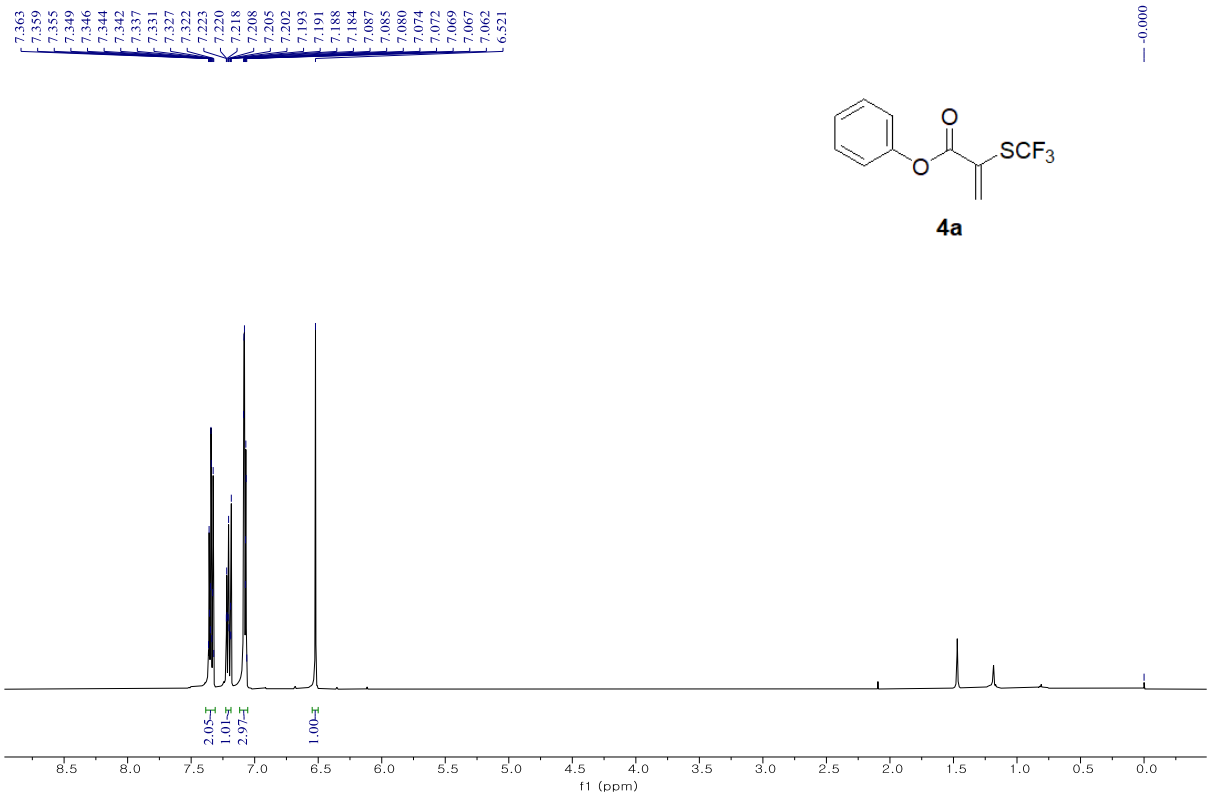
*[13]C NMR of **2s** (125 MHz, $CDCl_3$)*



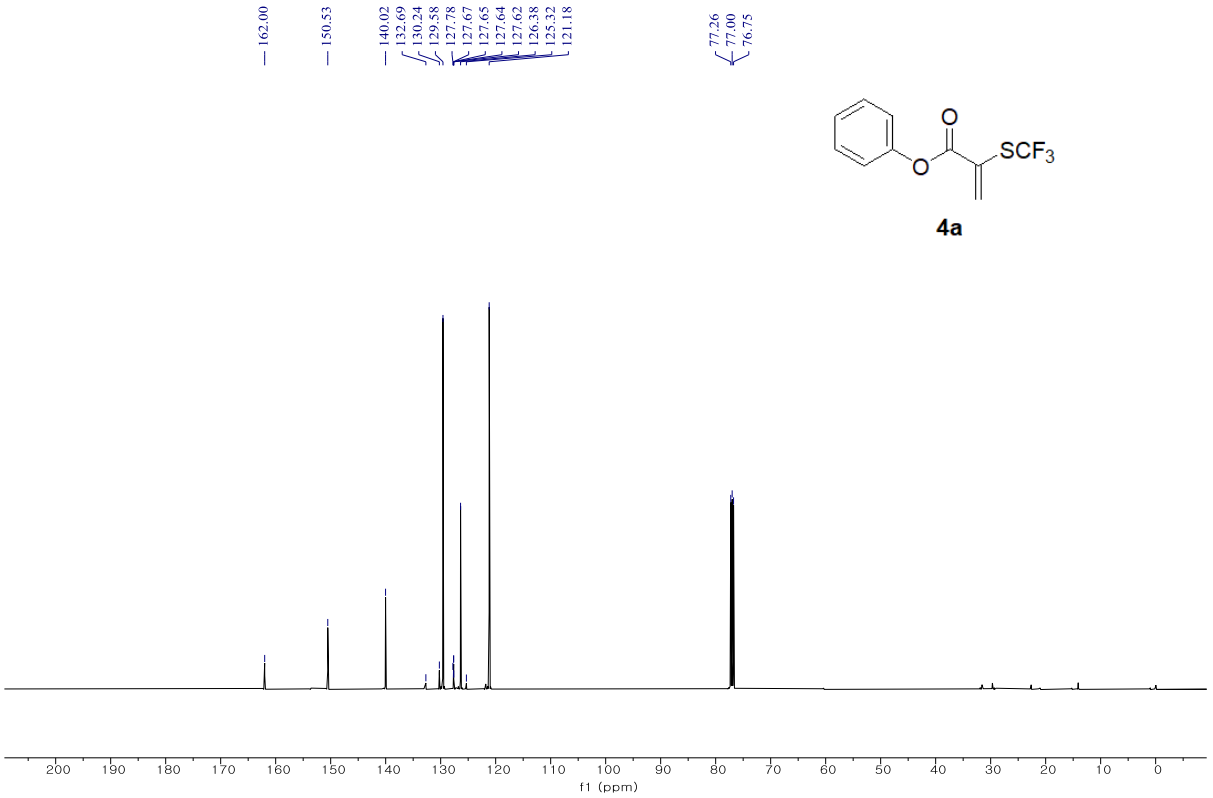
*^{19}F NMR of **2s** (564 MHz, $CDCl_3$)*



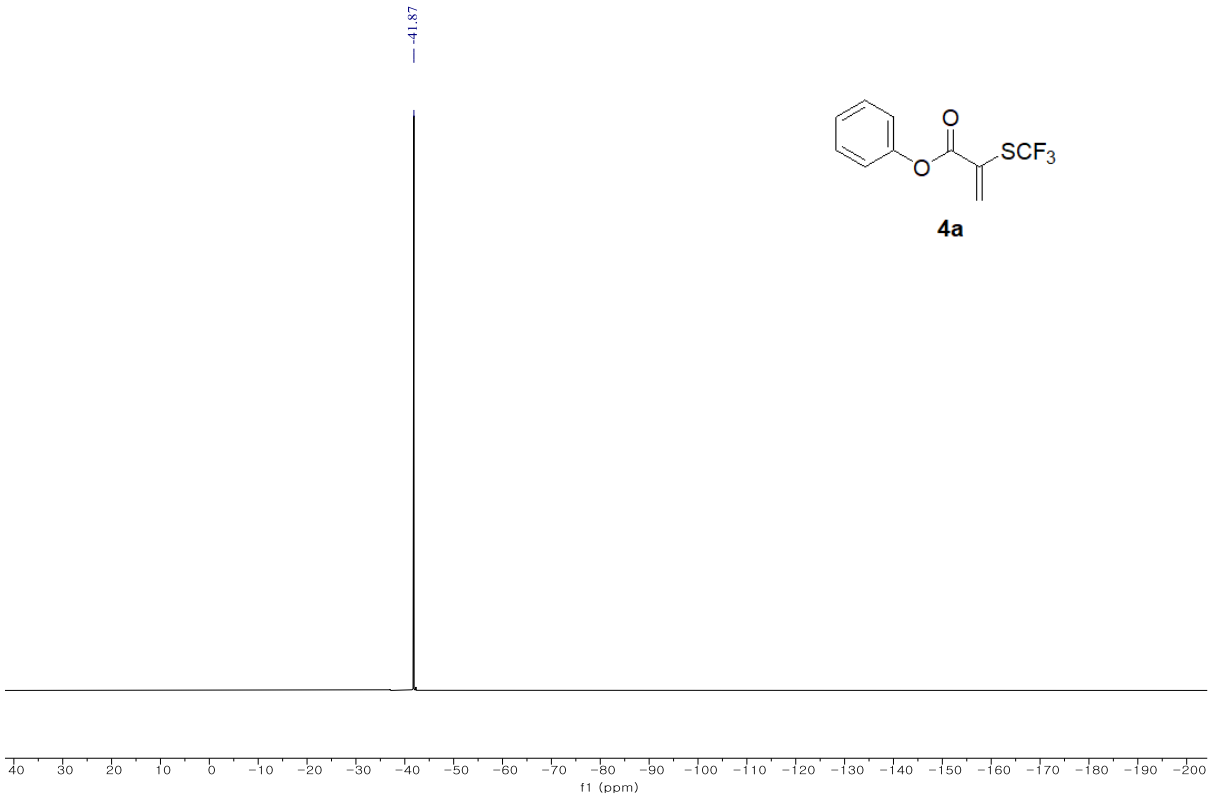
*^{1}H NMR of **4a** (500 MHz, $CDCl_3$)*



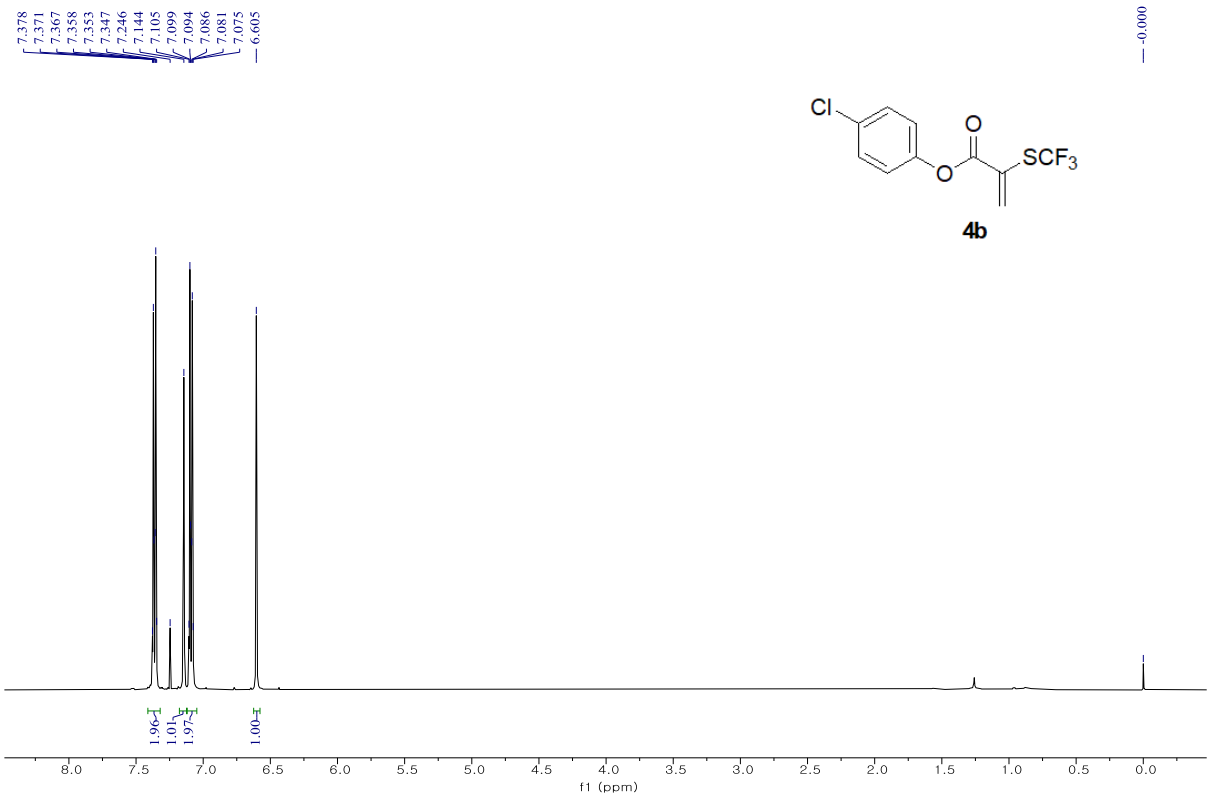
*^{13}C NMR of **4a** (125 MHz, $CDCl_3$)*



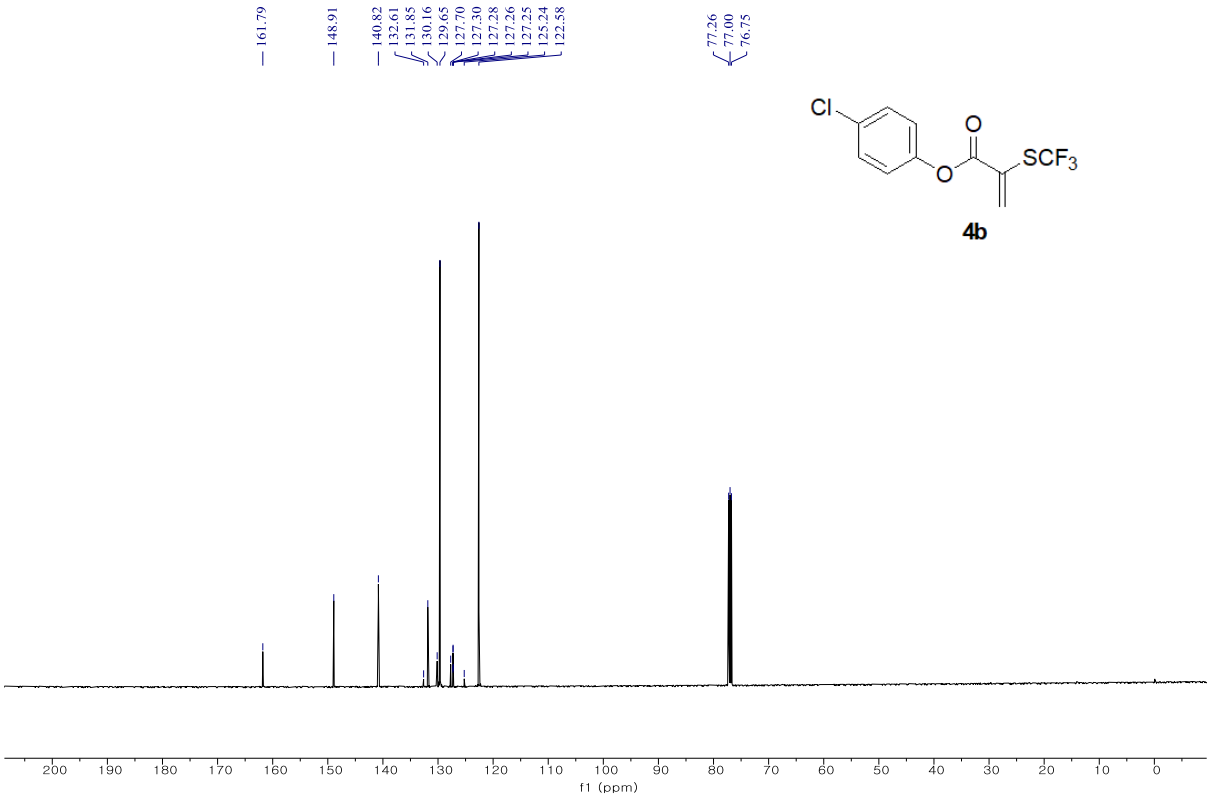
*^{19}F NMR of **4a** (564 MHz, $CDCl_3$)*



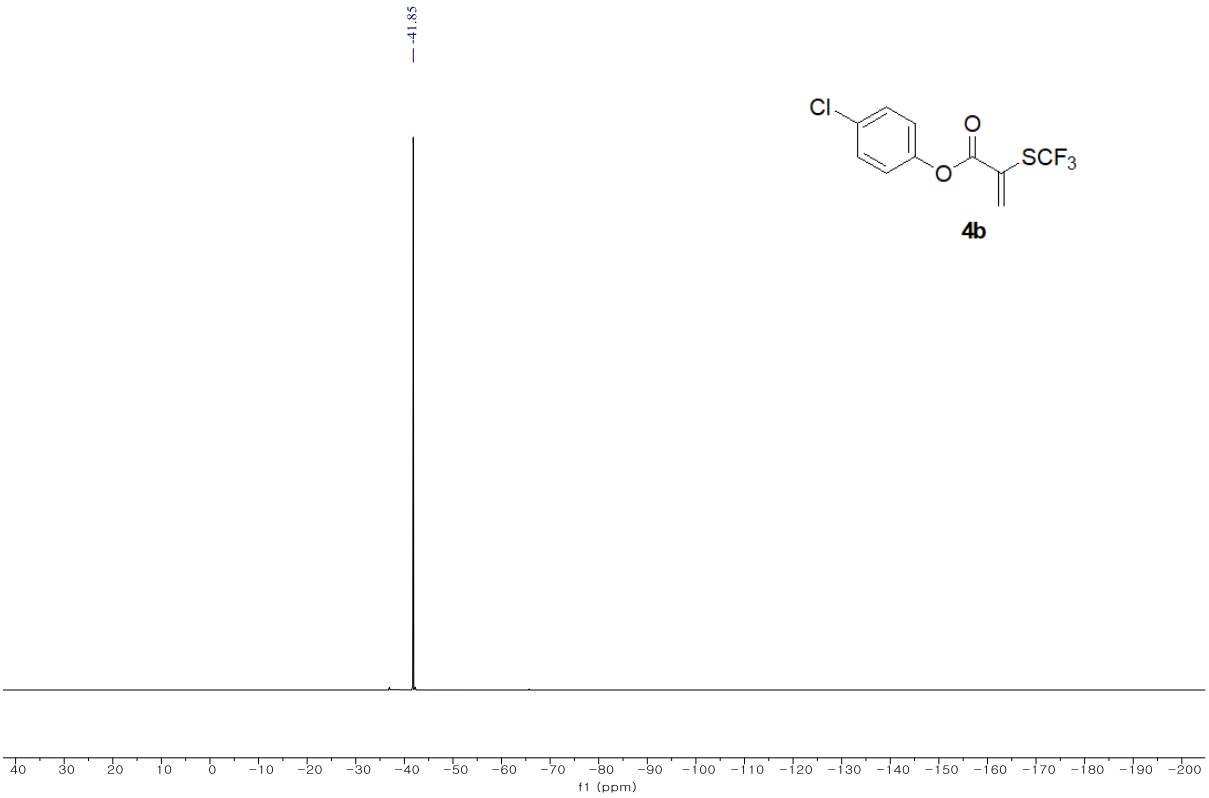
*[1]H NMR of **4b** (500 MHz, $CDCl_3$)*



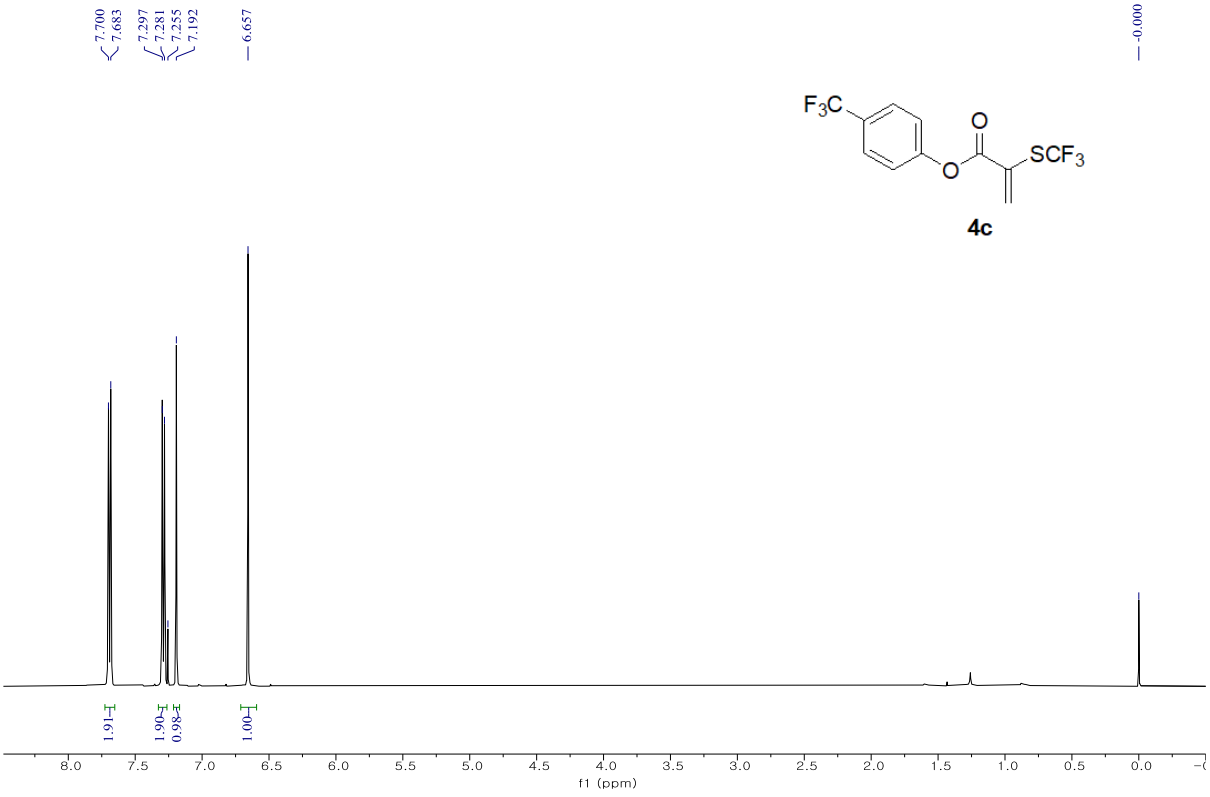
*[13]C NMR of **4b** (125 MHz, $CDCl_3$)*



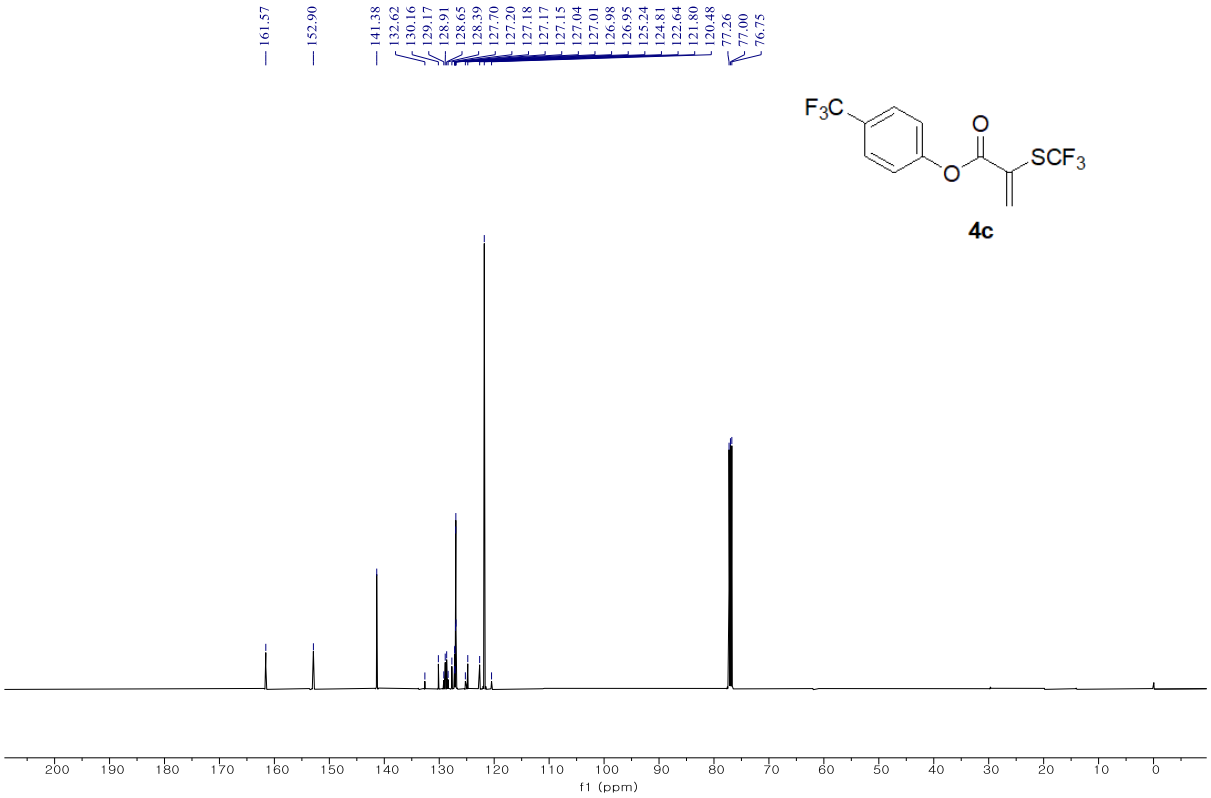
*^{19}F NMR of **4b** (564 MHz, $CDCl_3$)*



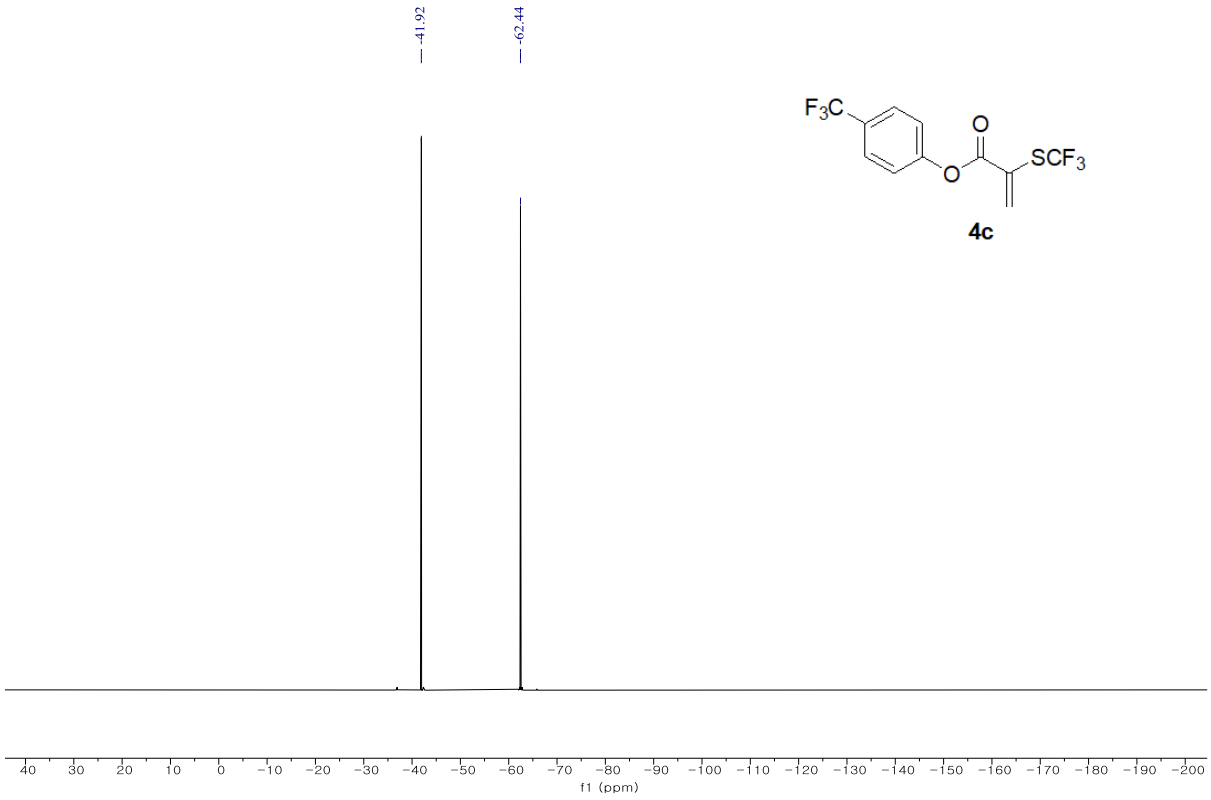
*^{1}H NMR of **4c** (500 MHz, $CDCl_3$)*



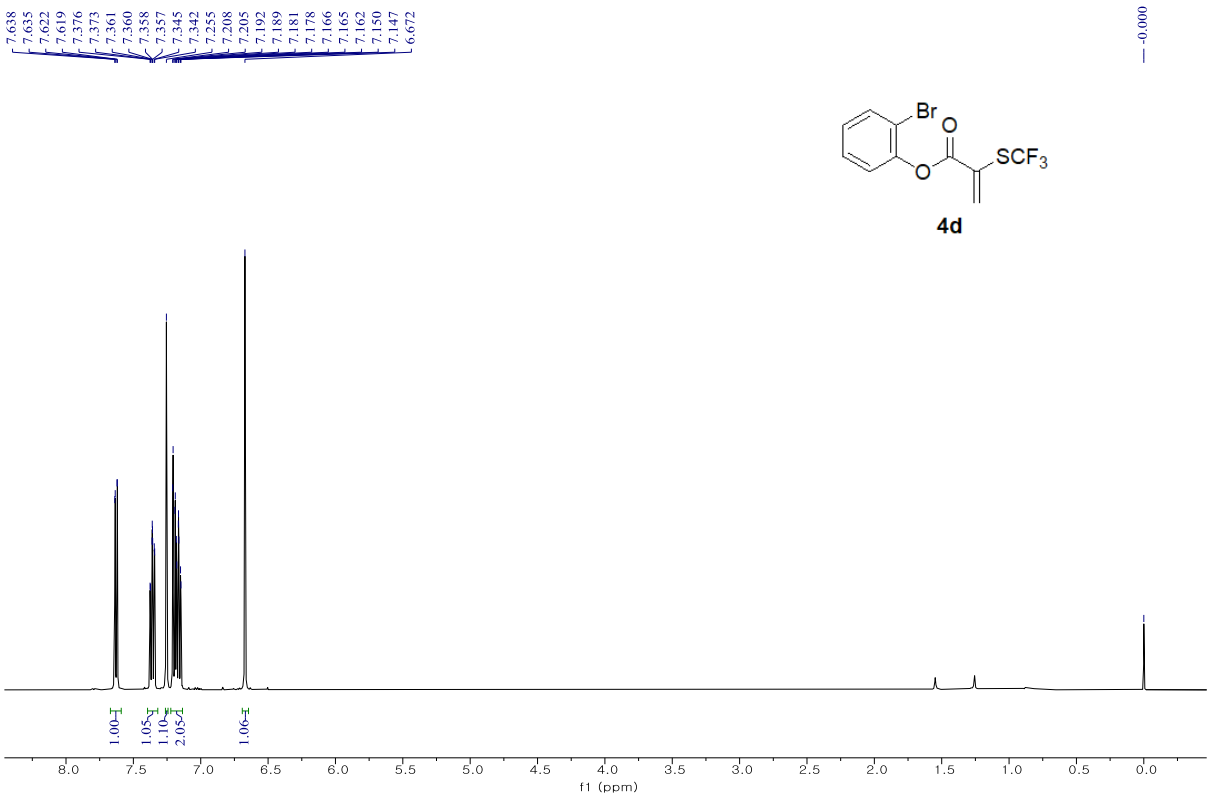
*^{13}C NMR of **4c** (125 MHz, $CDCl_3$)*



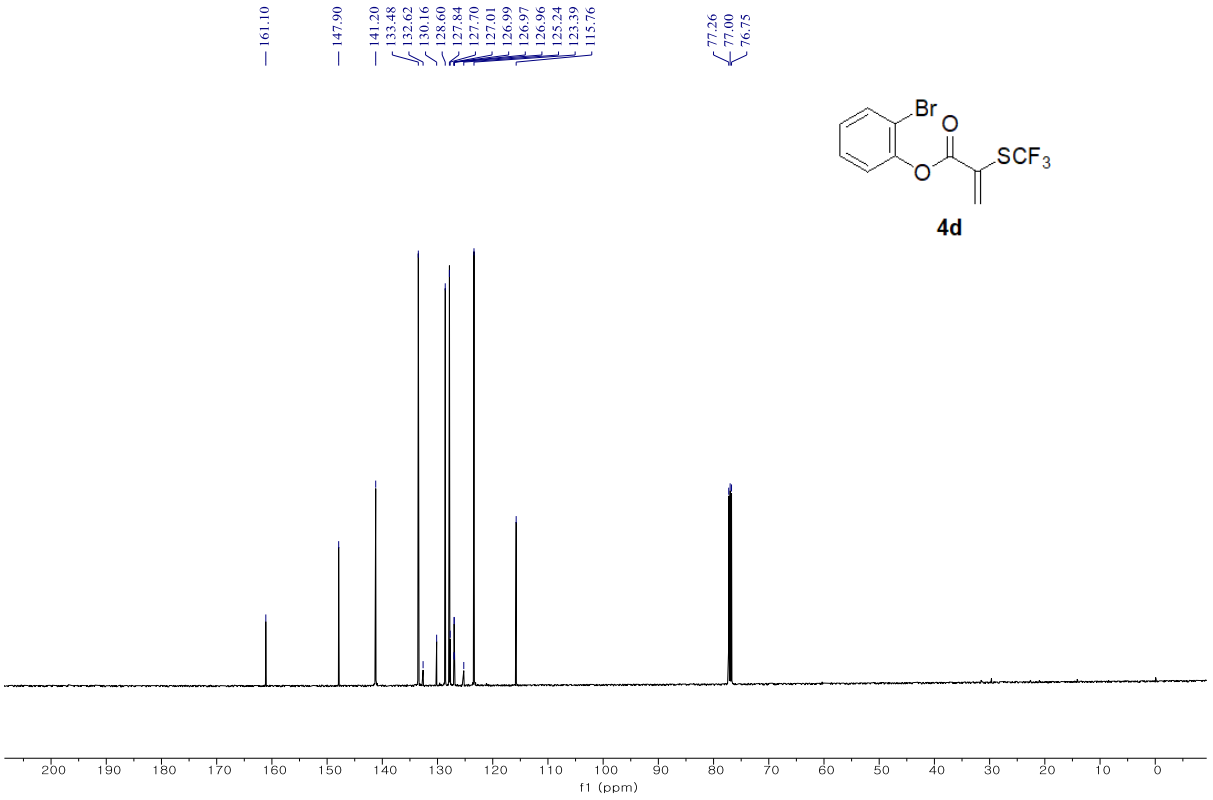
*^{19}F NMR of **4c** (564 MHz, $CDCl_3$)*



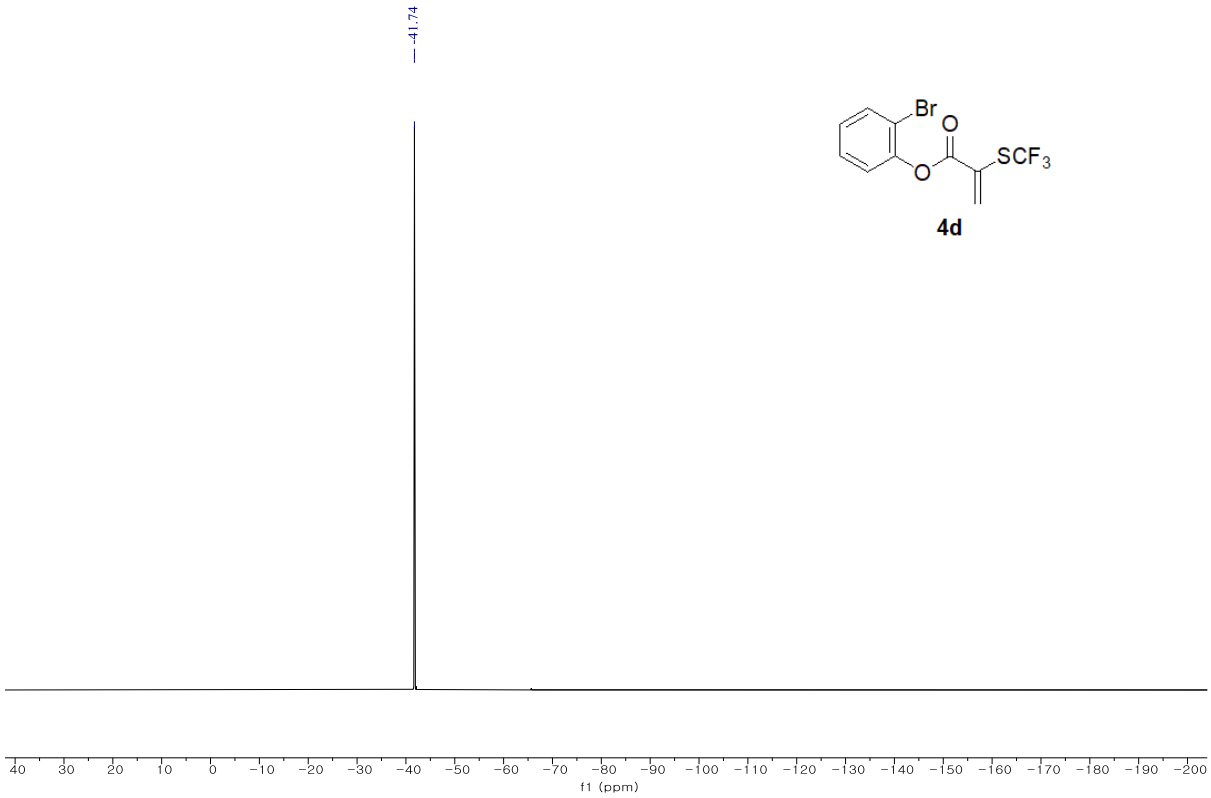
*[1]H NMR of **4d** (500 MHz, $CDCl_3$)*



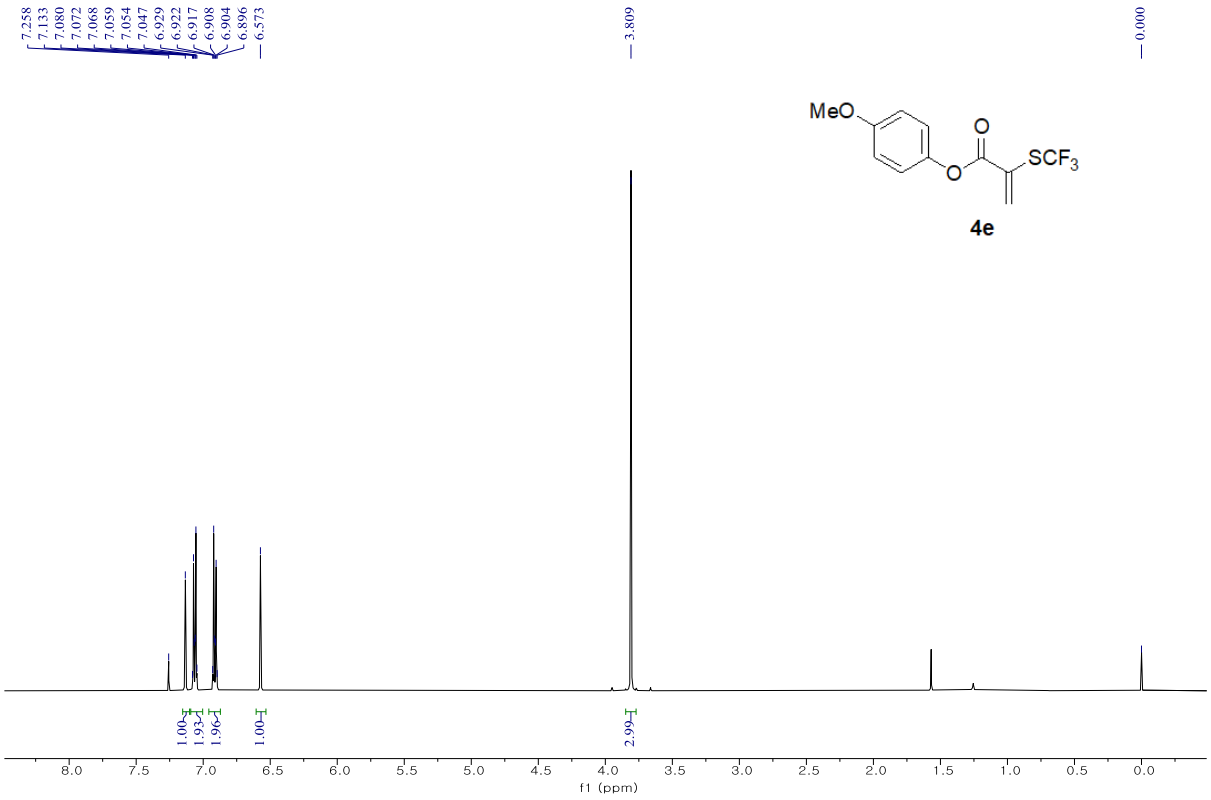
*[13]C NMR of **4d** (125 MHz, $CDCl_3$)*



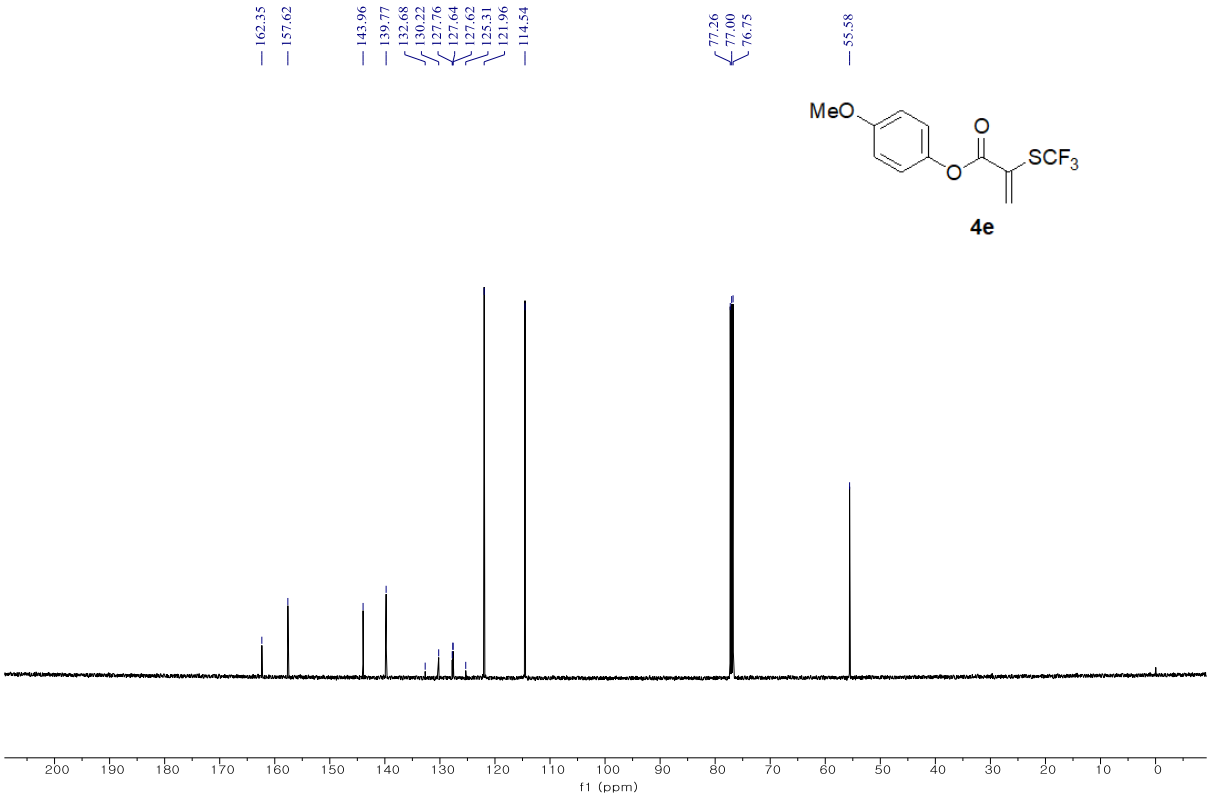
*^{19}F NMR of **4d** (564 MHz, $CDCl_3$)*



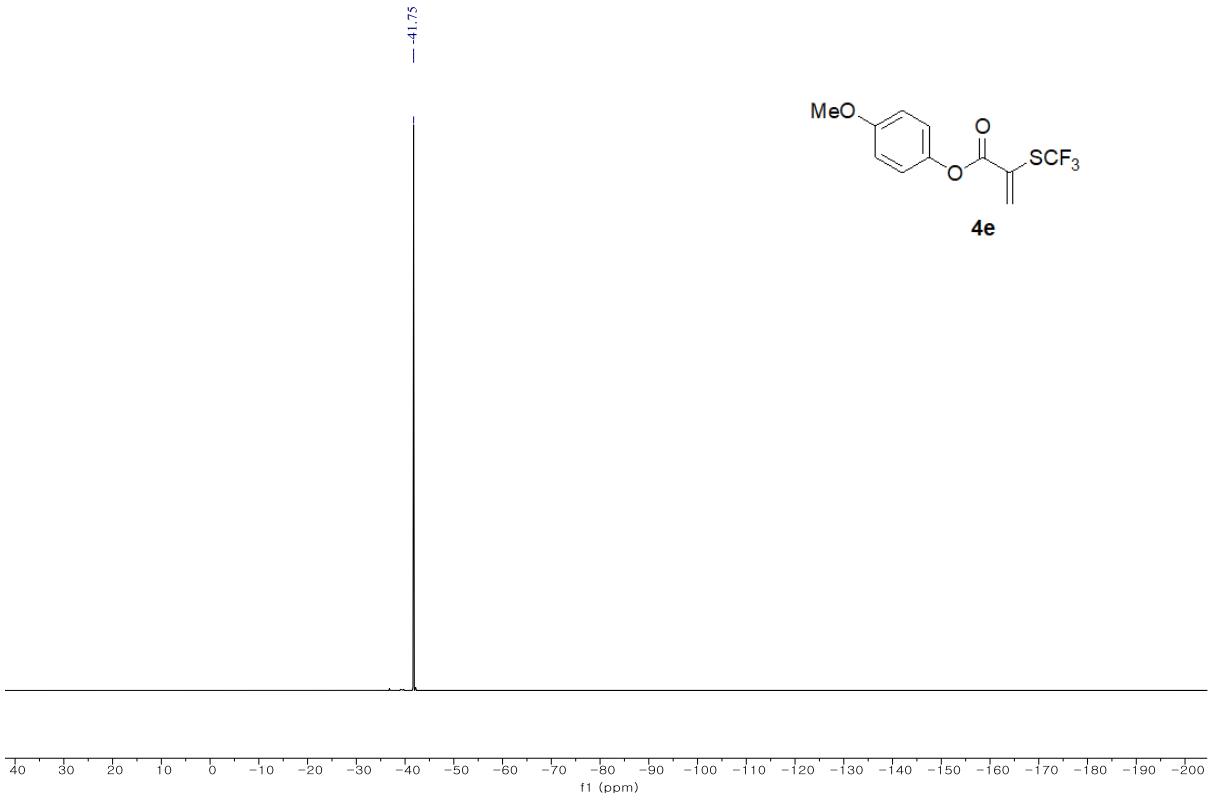
*^{1}H NMR of **4e** (500 MHz, $CDCl_3$)*



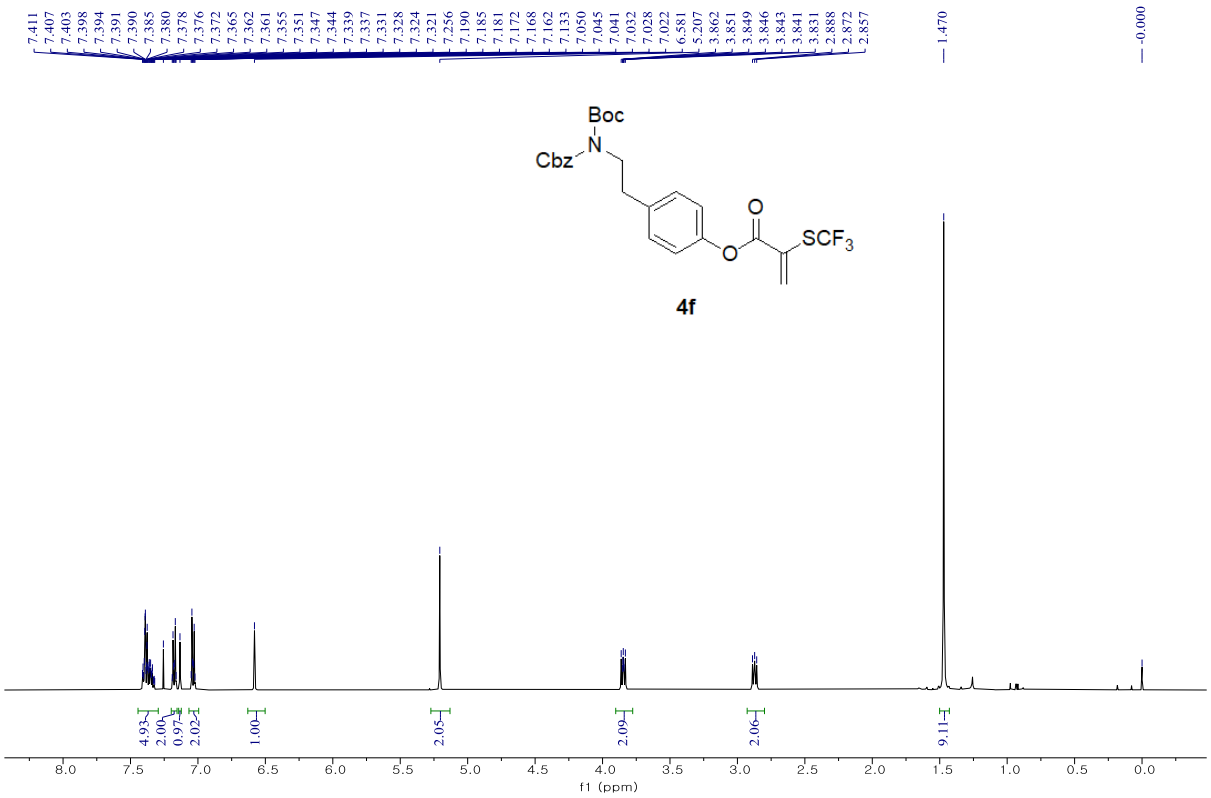
*^{13}C NMR of **4e** (125 MHz, $CDCl_3$)*



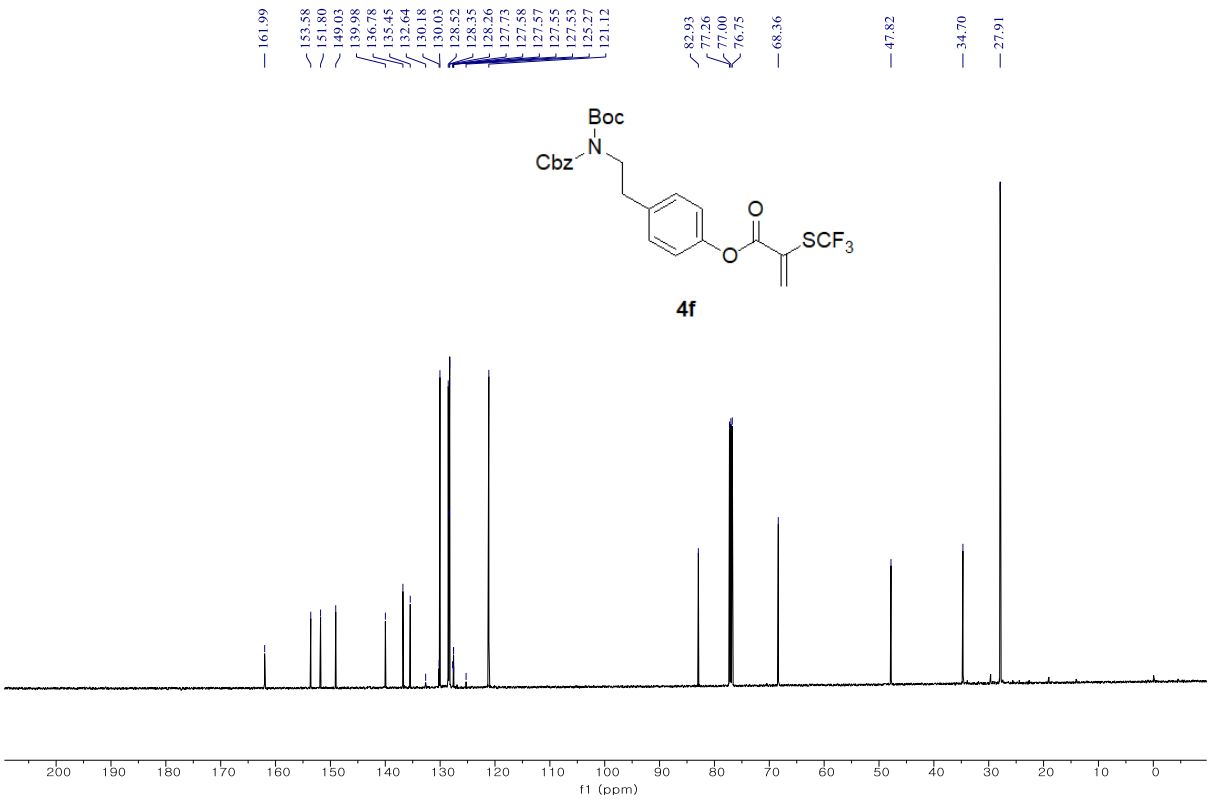
*^{19}F NMR of **4e** (564 MHz, $CDCl_3$)*



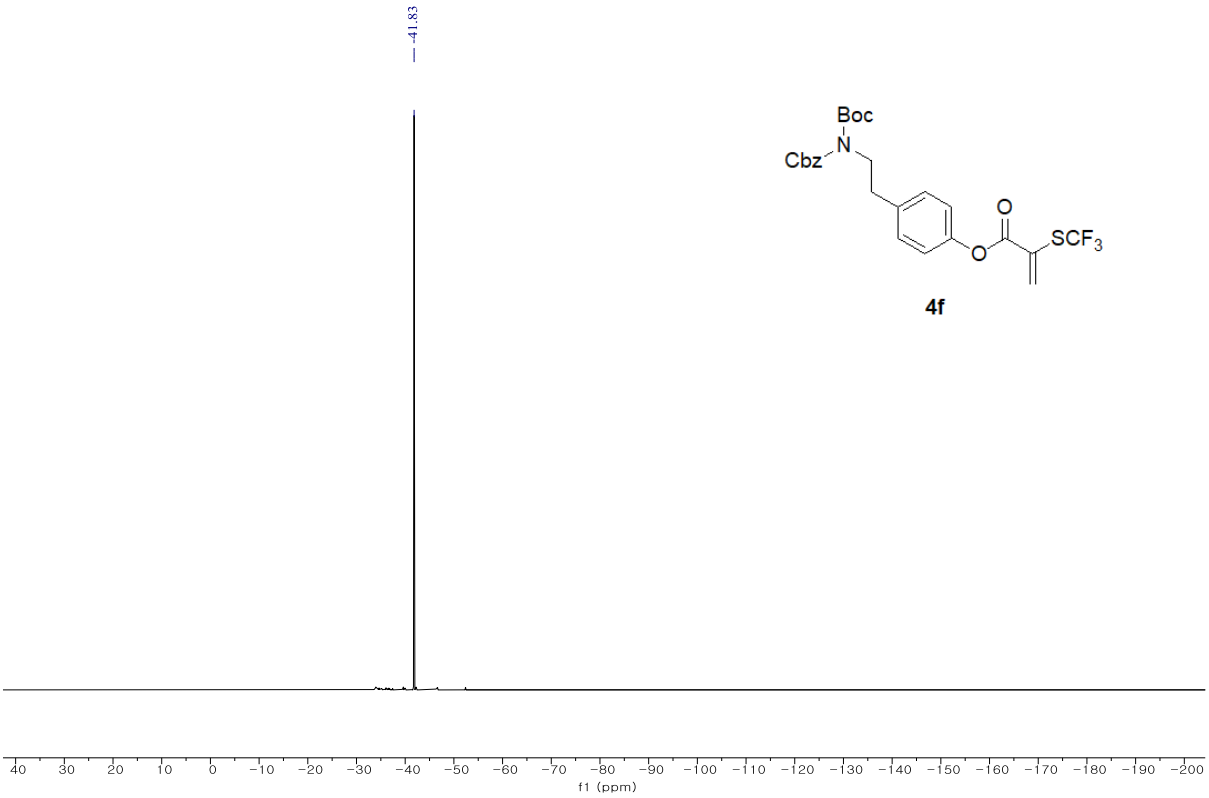
*[1]H NMR of **4f** (500 MHz, $CDCl_3$)*



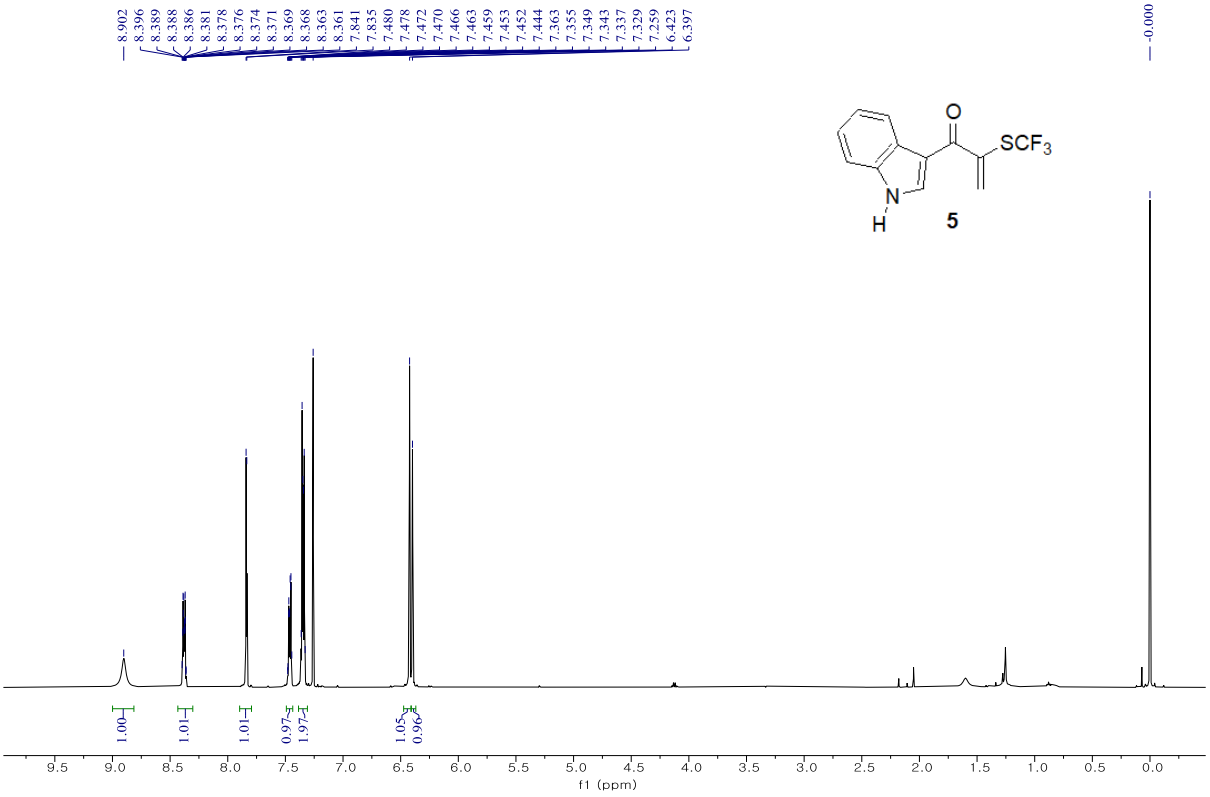
*[13]C NMR of **4f** (125 MHz, $CDCl_3$)*



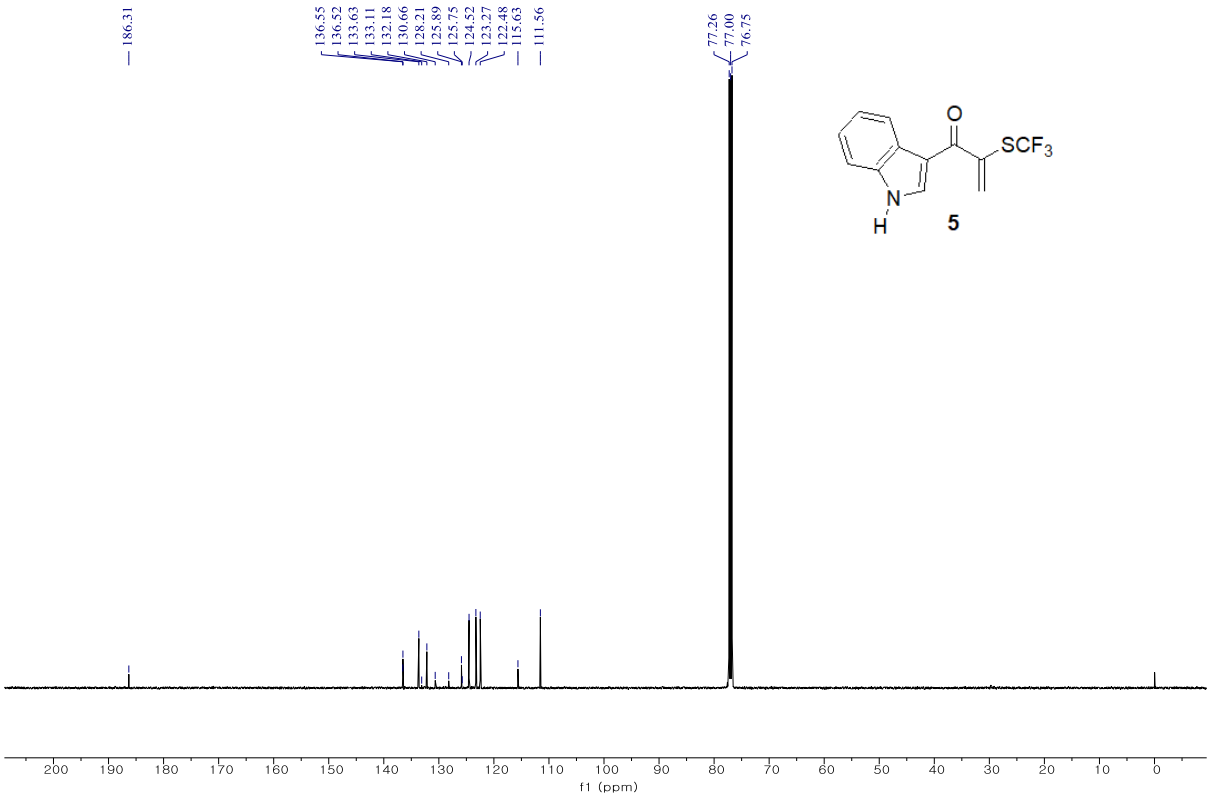
*^{19}F NMR of **4f** (564 MHz, $CDCl_3$)*



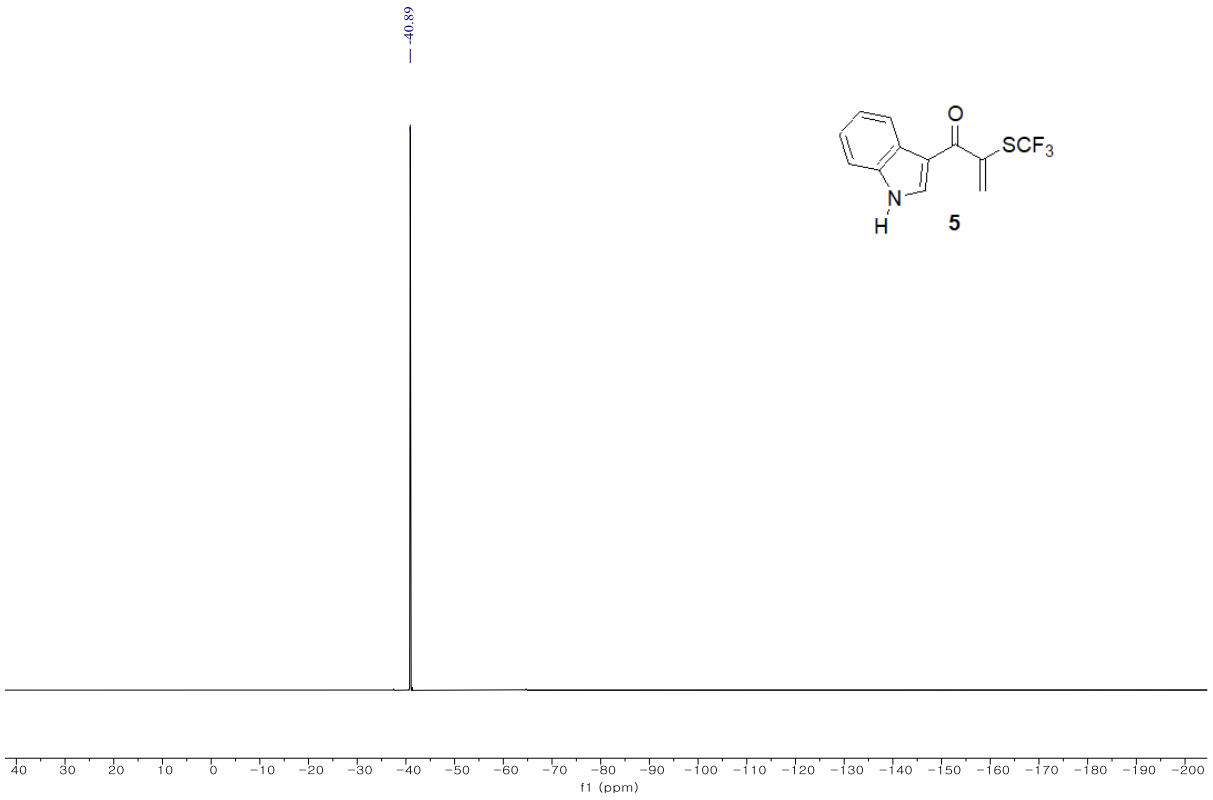
*^{1}H NMR of **5** (500 MHz, $CDCl_3$)*



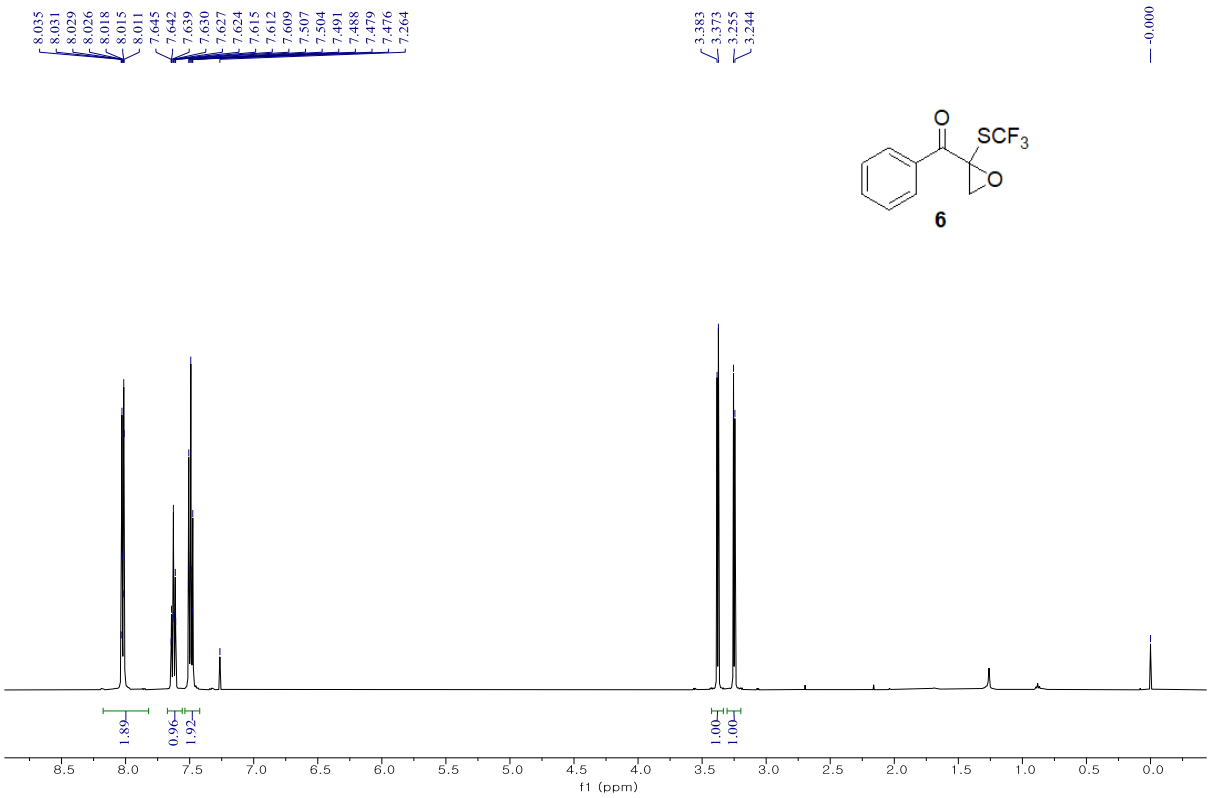
*^{13}C NMR of **5** (125 MHz, $CDCl_3$)*



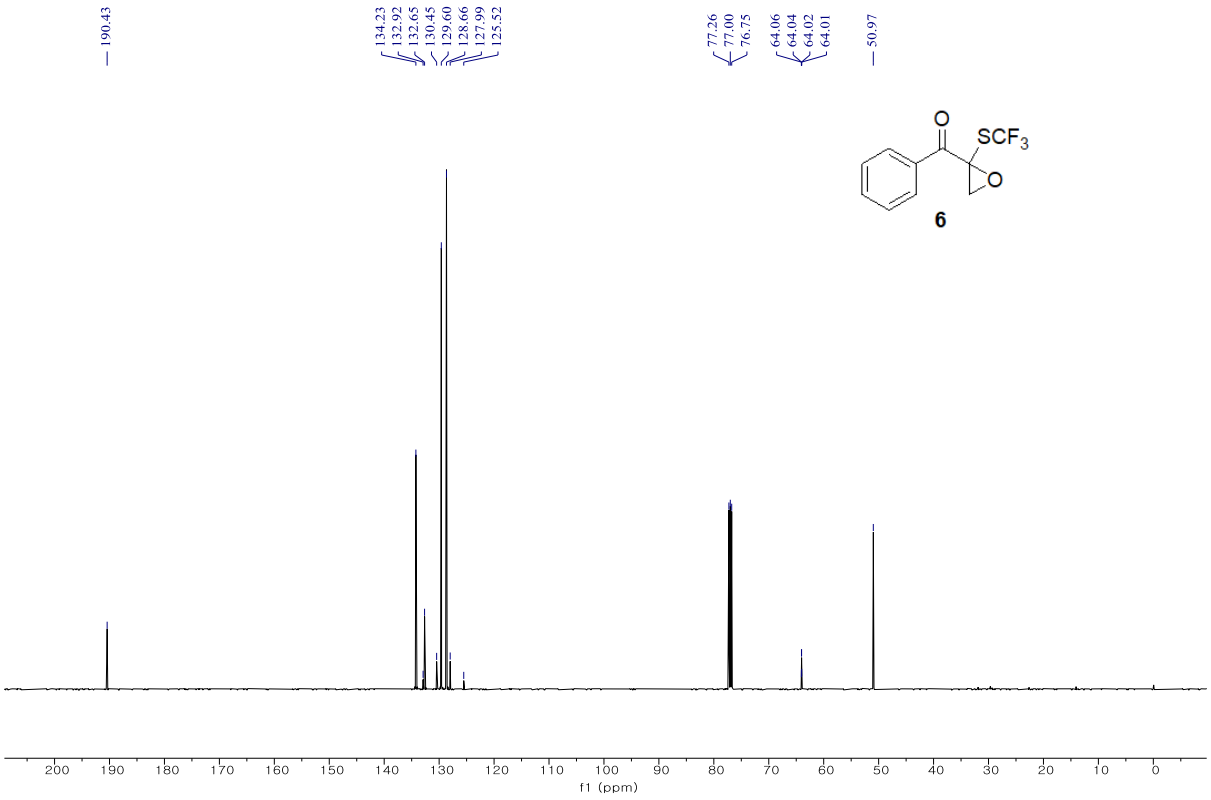
*^{19}F NMR of **5** (564 MHz, $CDCl_3$)*



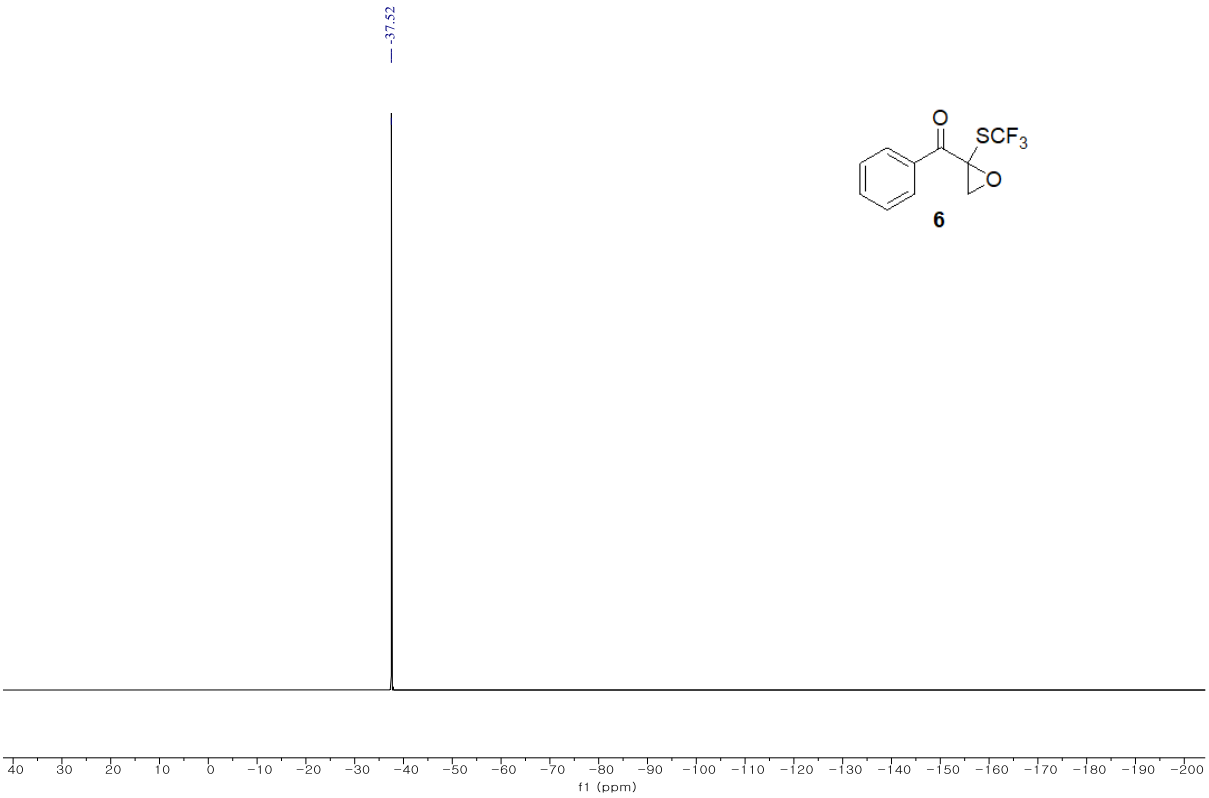
*[1]H NMR of **6** (500 MHz, CDCl3)*



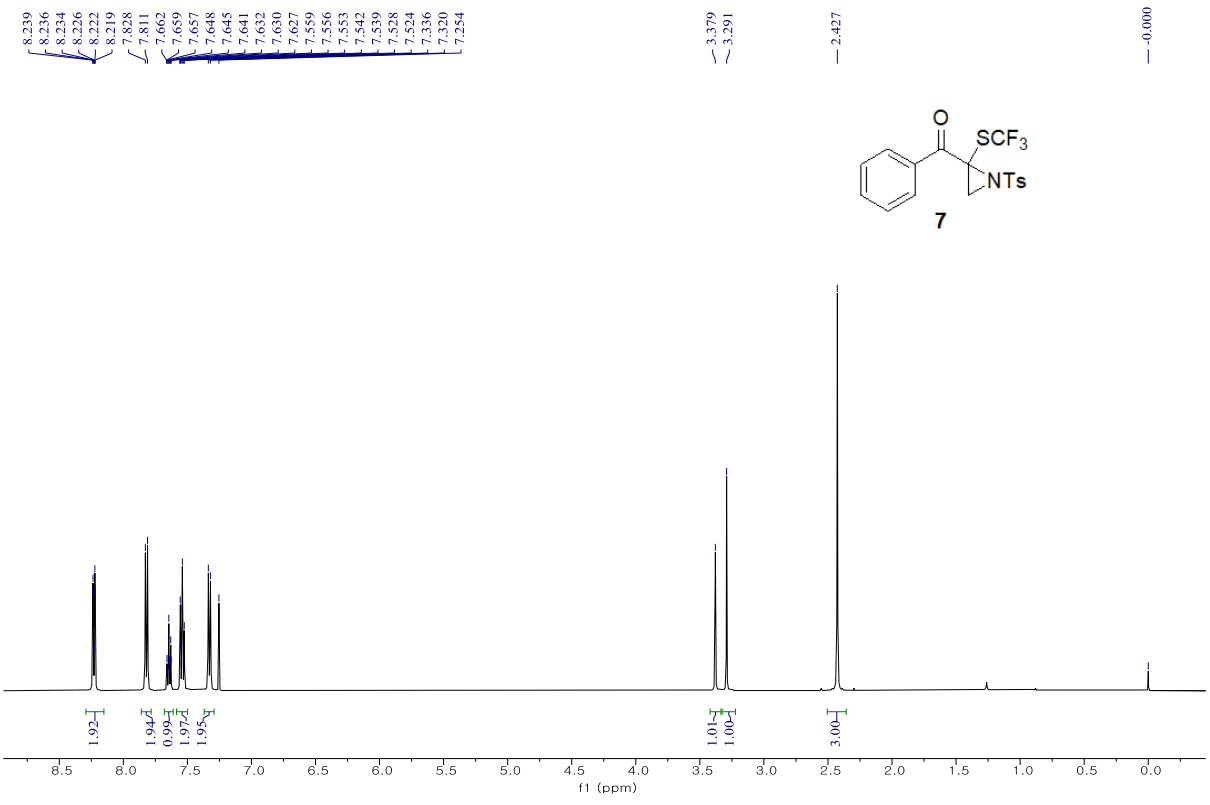
*[13]C NMR of **6** (125 MHz, CDCl3)*



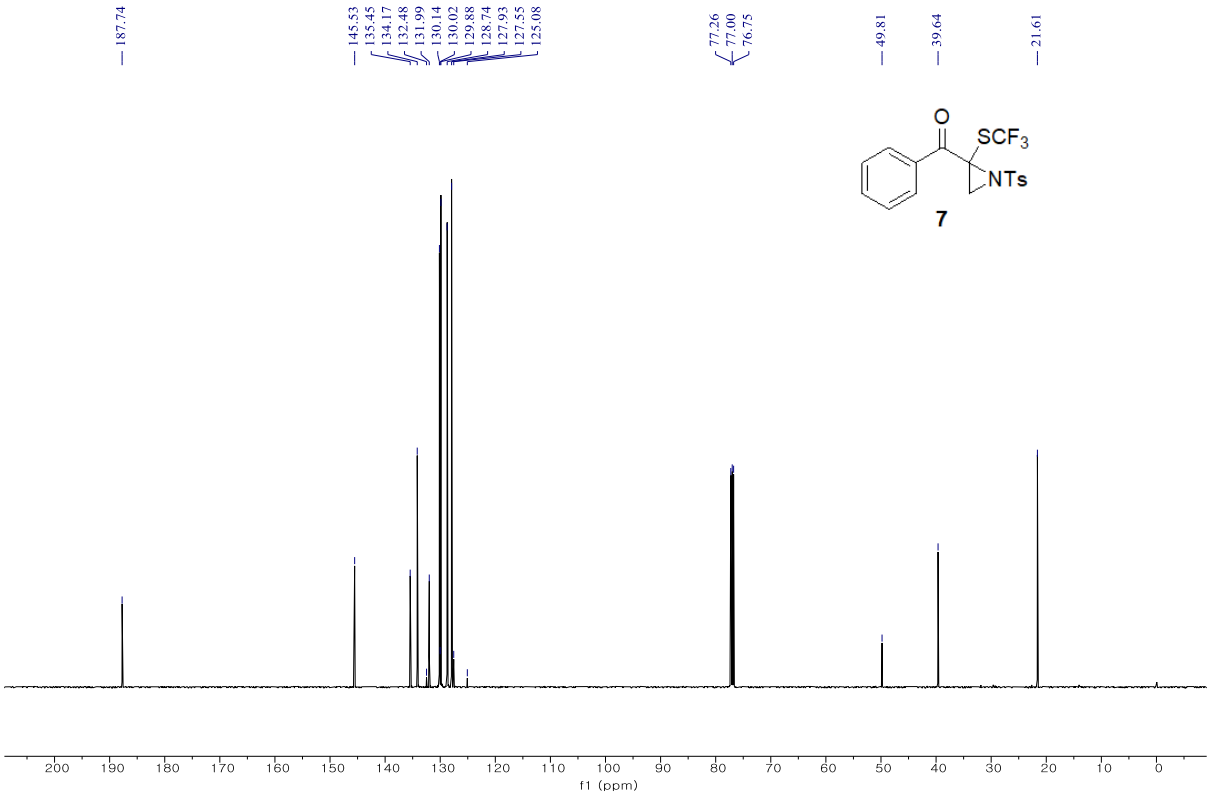
*^{19}F NMR of **6** (564 MHz, $CDCl_3$)*



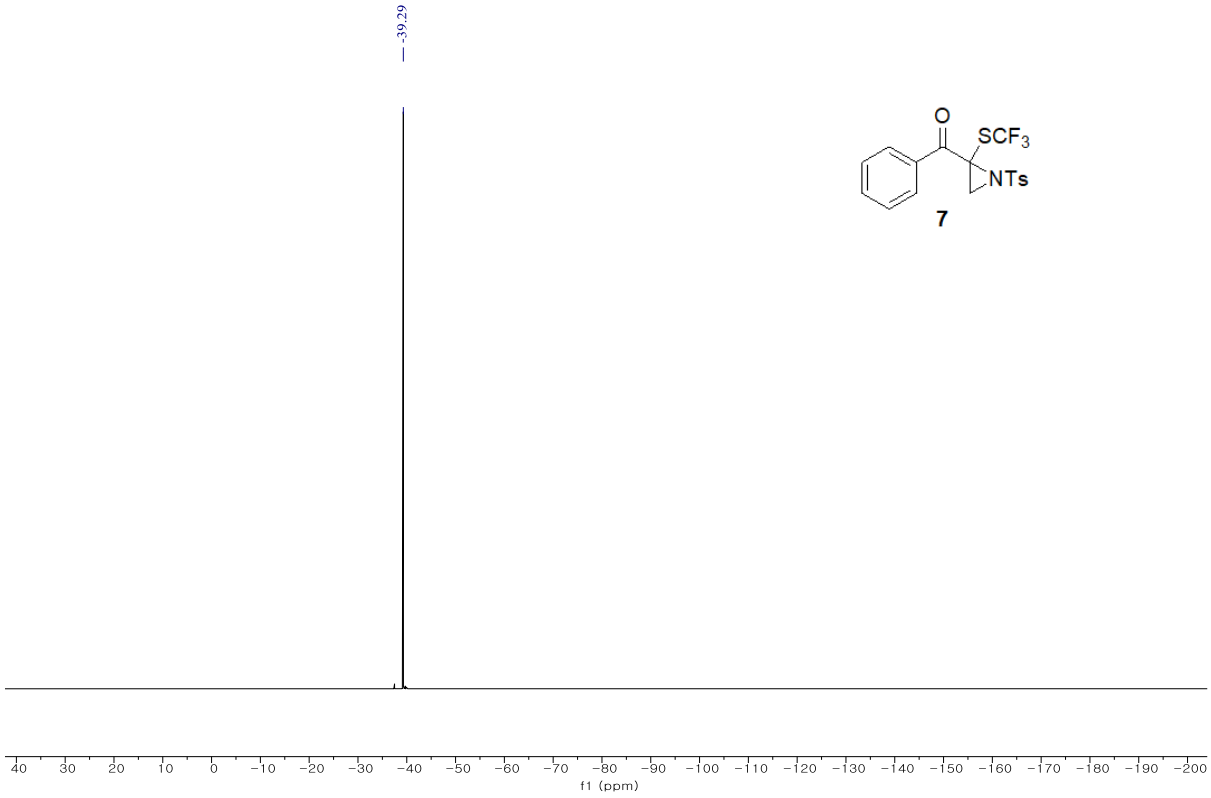
*^{1}H NMR of **7** (500 MHz, $CDCl_3$)*



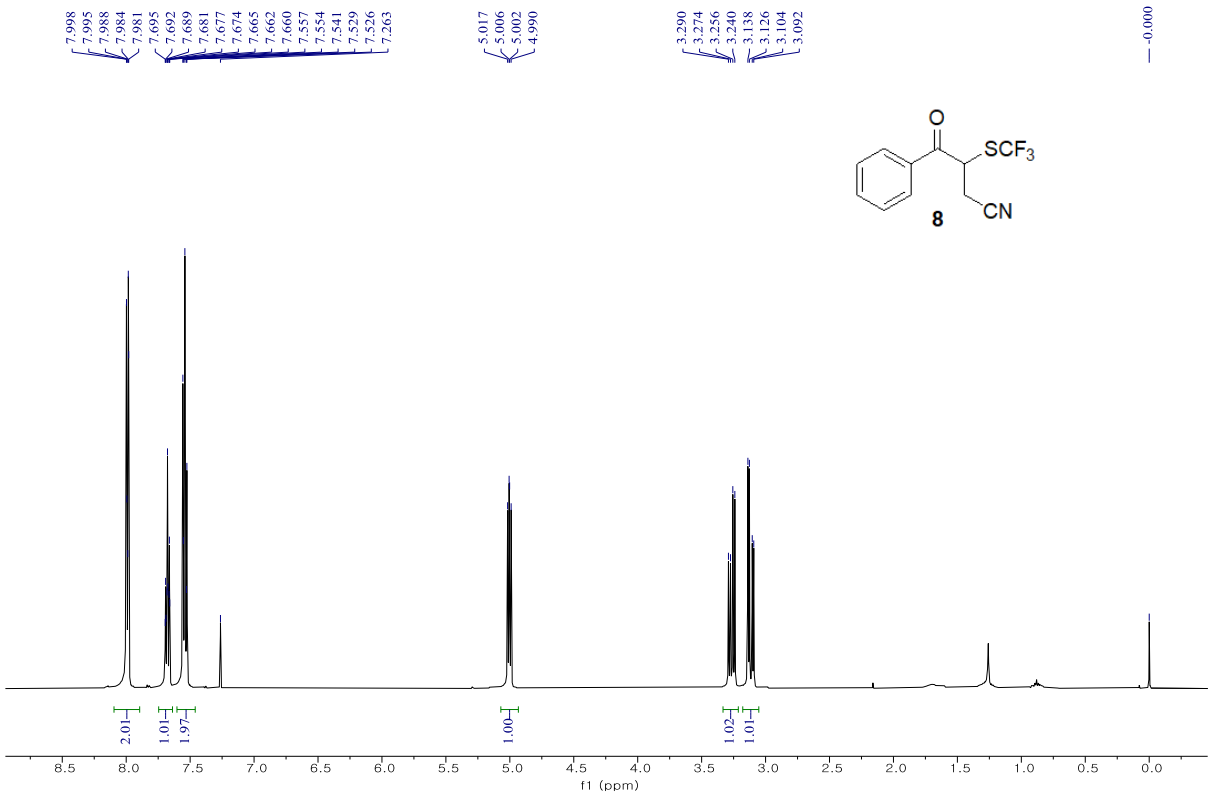
^{13}C NMR of 7 (125 MHz, $CDCl_3$)



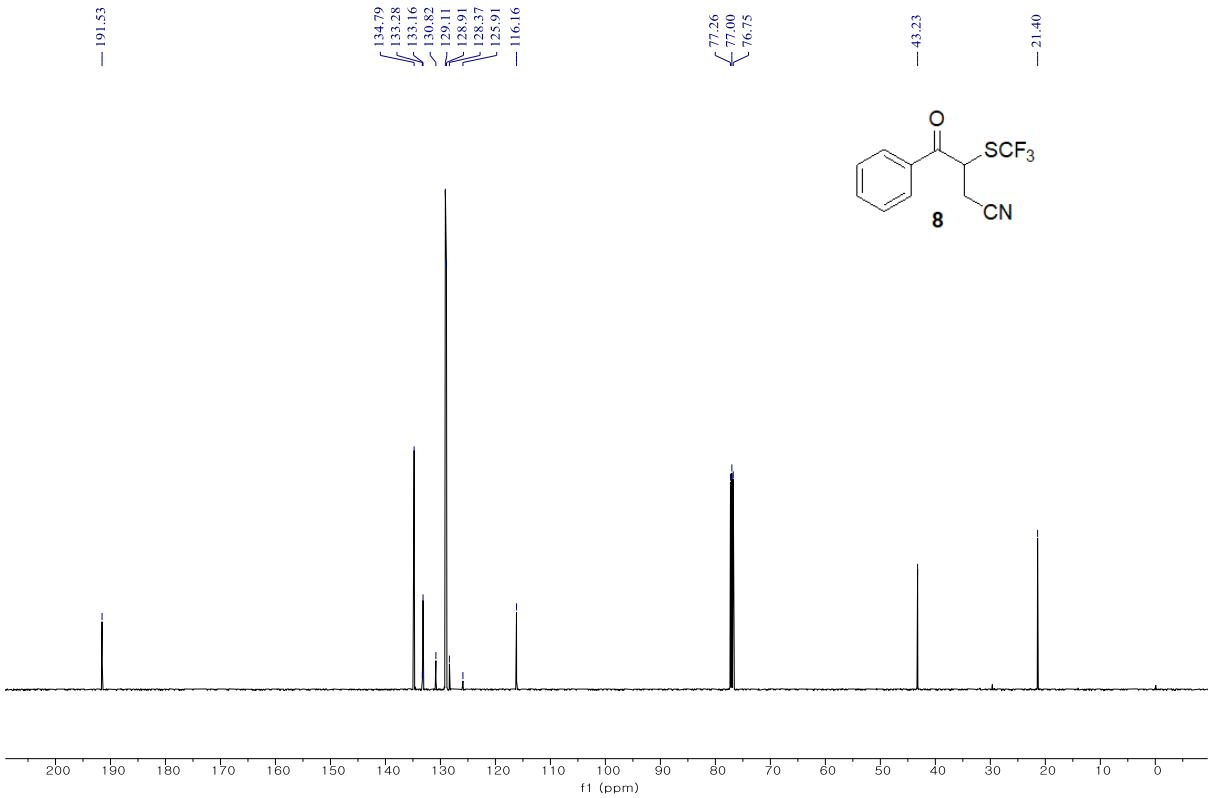
^{19}F NMR of 7 (564 MHz, $CDCl_3$)



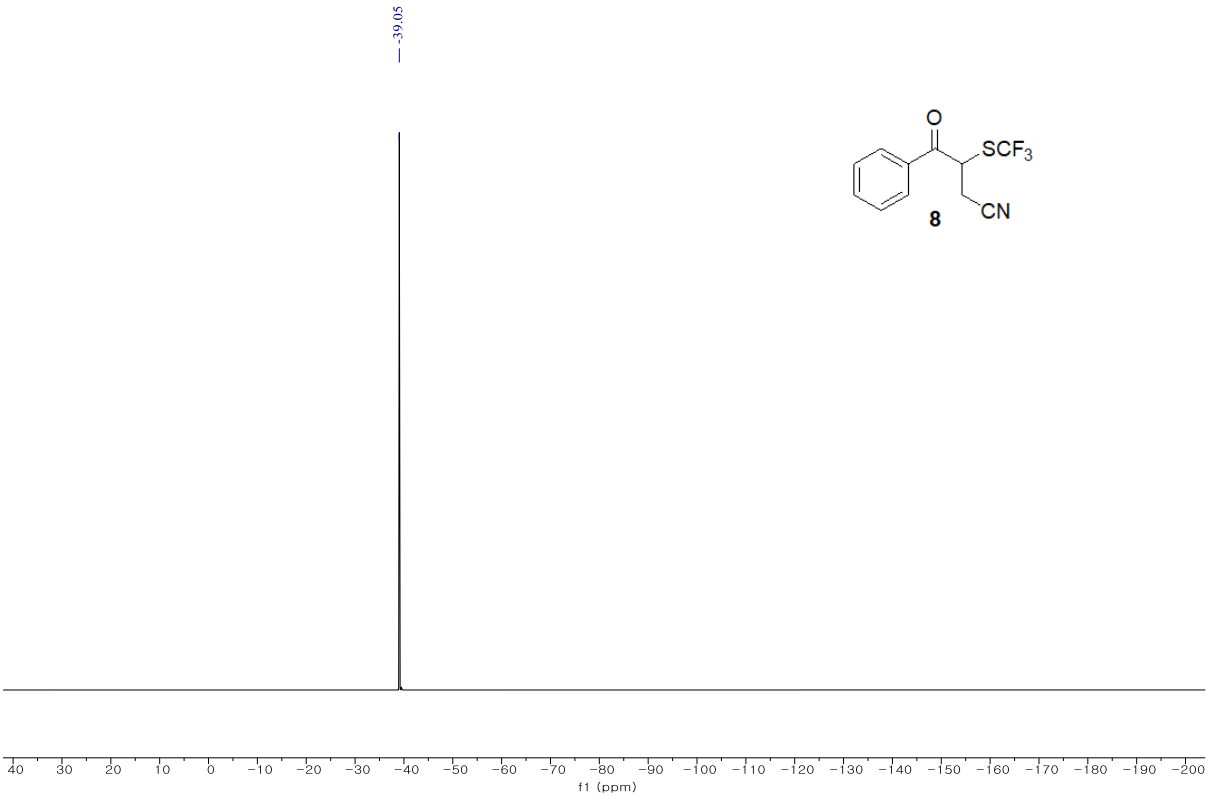
*[1]H NMR of **8** (500 MHz, $CDCl_3$)*



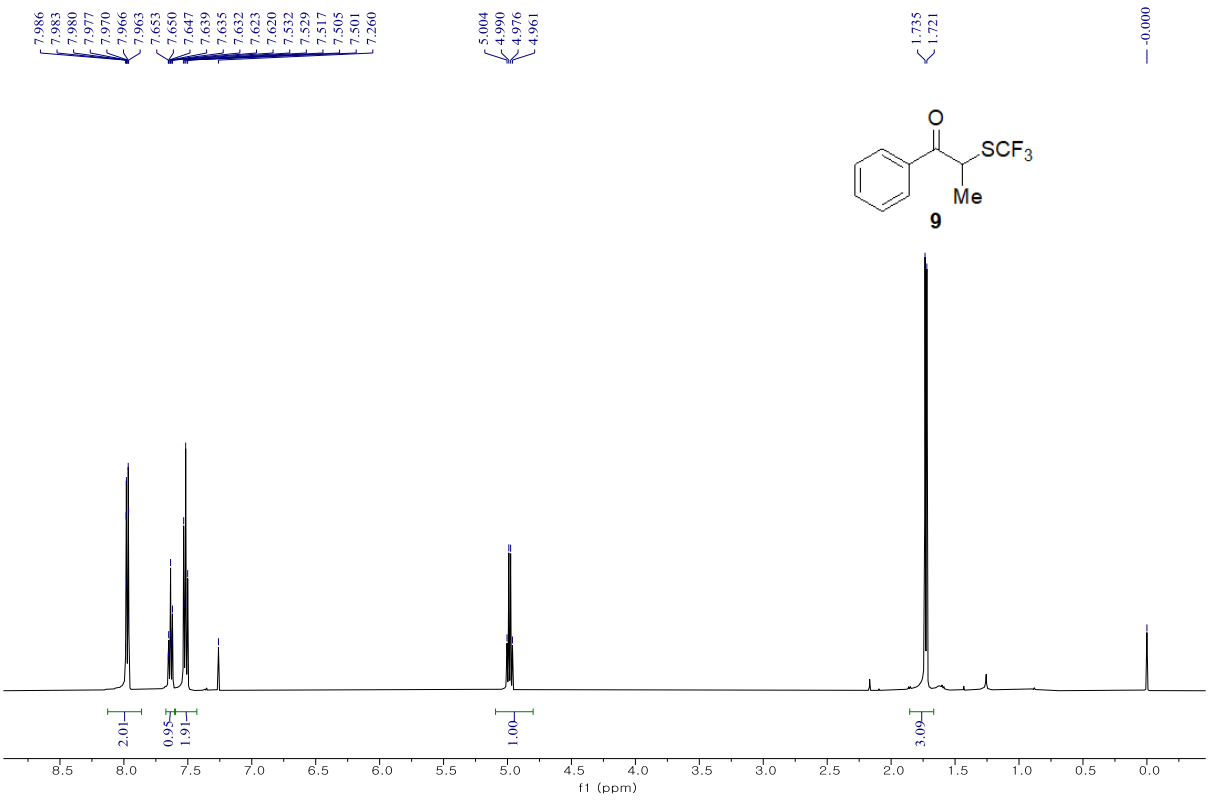
*[13]C NMR of **8** (125 MHz, $CDCl_3$)*



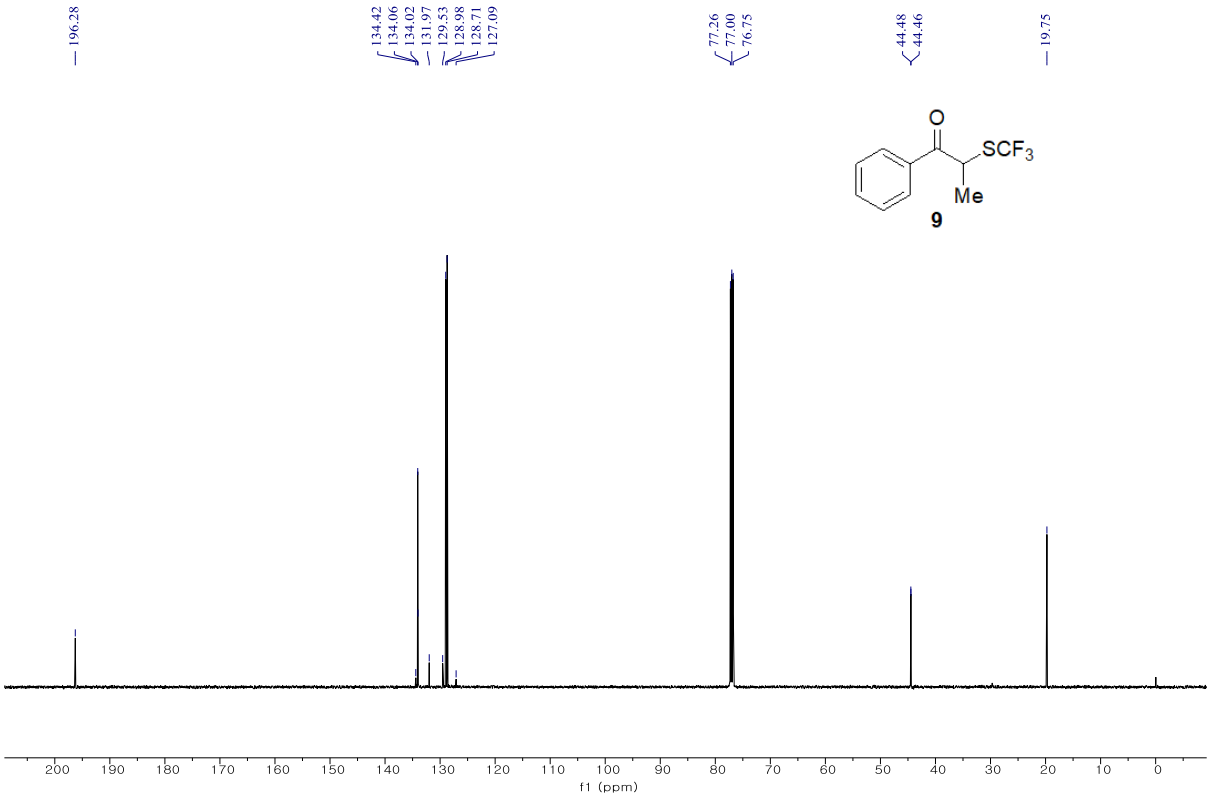
*^{19}F NMR of **8** (564 MHz, $CDCl_3$)*



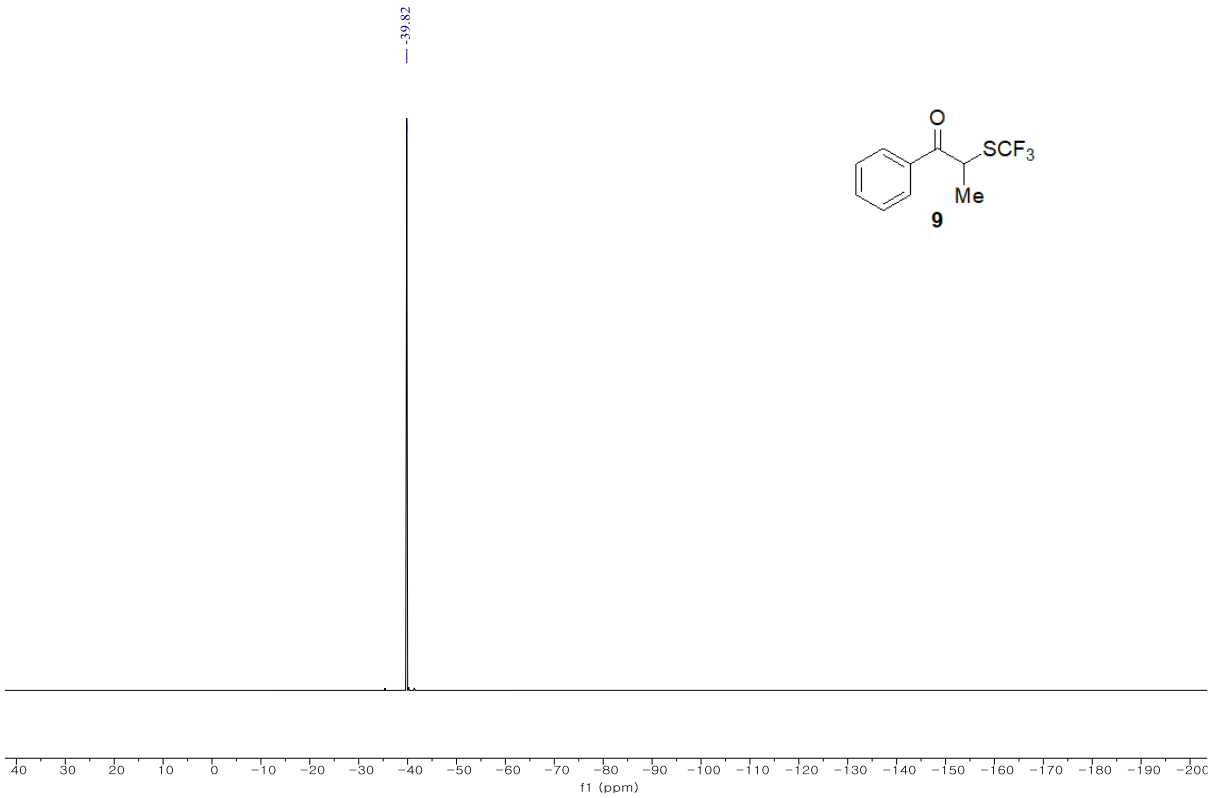
*^{1}H NMR of **9** (500 MHz, $CDCl_3$)*



*^{13}C NMR of **9** (125 MHz, $CDCl_3$)*



*^{19}F NMR of **9** (564 MHz, $CDCl_3$)*



X-Ray crystallographic data of compound 5

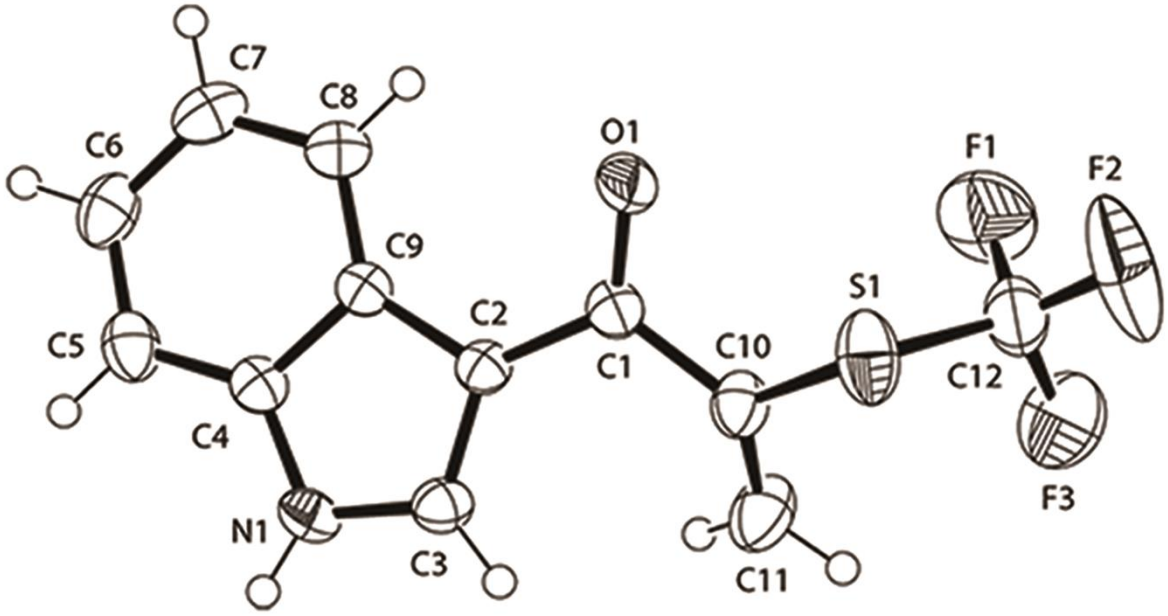


Figure S1. X-Ray crystal structure of **5**. Thermal ellipsoids are drawn at the 50% probability level.

Sample preparation

A single crystal of compound **5** was obtained by slow evaporation of a solution of **5** in dichloromethane–hexanes at room temperature.

Table S1. Crystal data and structure refinement for **5**

Identification code	**5**	
Empirical formula	C12 H8 F3 N O S	
Formula weight	271.25	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 8.2239(10) Å	α= 90°.
	b = 11.2158(11) Å	β= 90°.
	c = 25.146(3) Å	γ = 90°.
Volume	2319.4(5) $Å^3$	
Z	8	
Density (calculated)	1.554 Mg/m^3	
Absorption coefficient	0.304 mm^{-1}	
F(000)	1104	
Crystal size	0.230 x 0.150 x 0.050 mm^3	
Theta range for data collection	2.960 to 28.376°.	
Index ranges	-10<=h<=10, -14<=k<=14, -33<=l<=33	
Reflections collected	72285	
Independent reflections	2893 [R(int) = 0.0777]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6950	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2893 / 0 / 163	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0588, wR2 = 0.1393	
R indices (all data)	R1 = 0.0823, wR2 = 0.1554	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.103 and -0.607 $e.Å^{-3}$	