

## Supporting Information

# Synthesis of Allenyl Sulfones *via* a TBHP/TBAI-Mediated Reaction of Propargyl Alcohols with Sulfonyl Hydrazides

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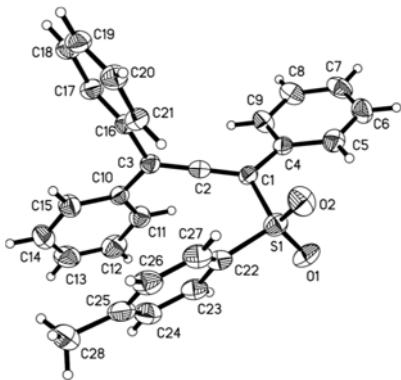
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## Context

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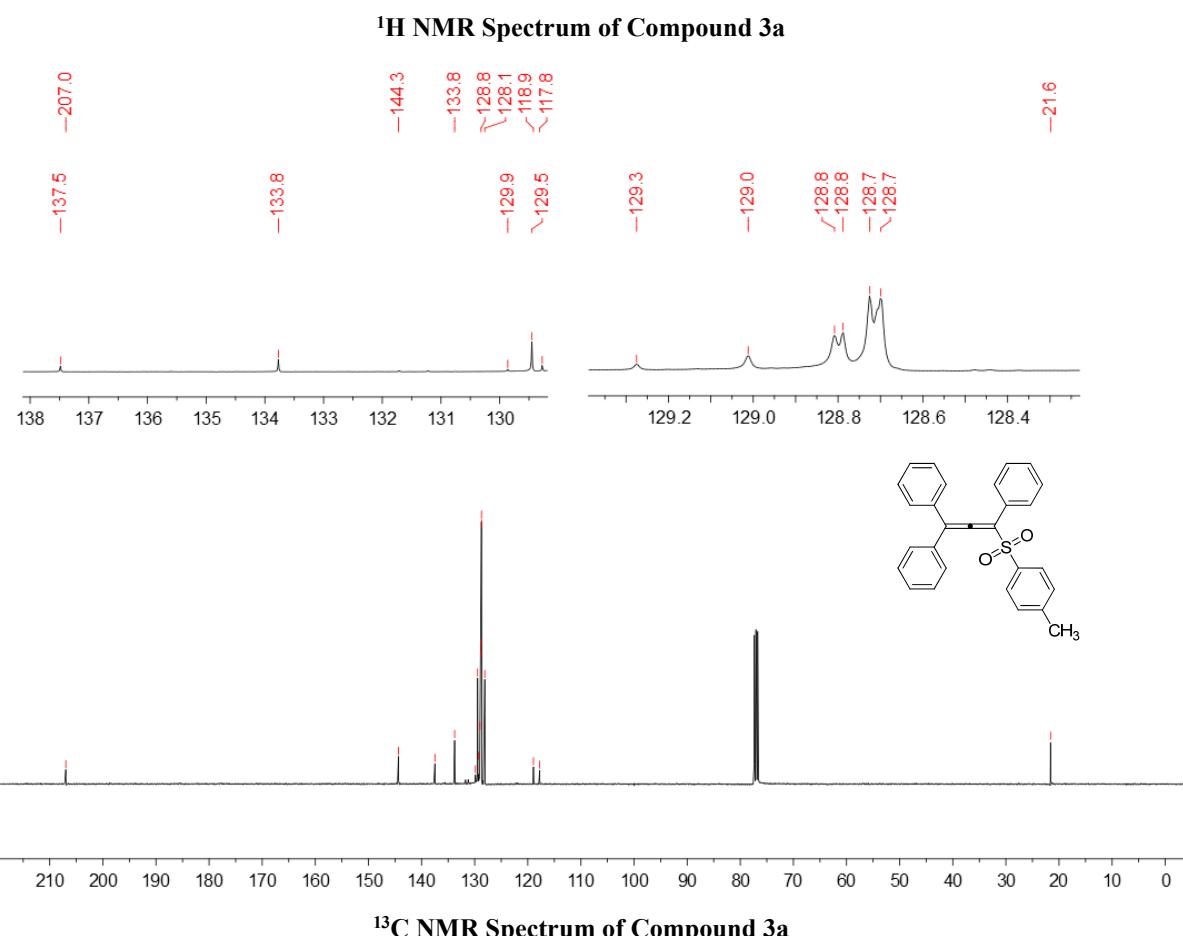
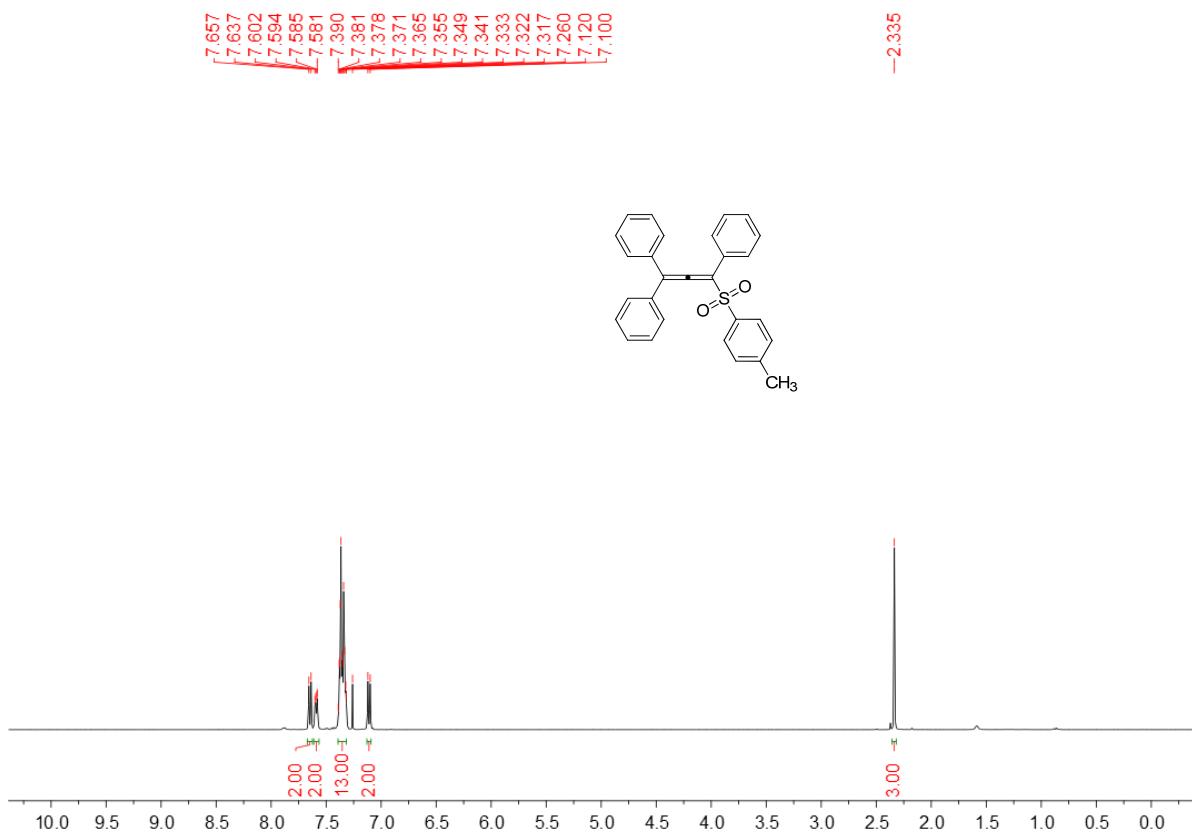
**Figure 1** The ORTEP Drawing of **3a** (Thermal ellipsoids are set at 30% probability level)

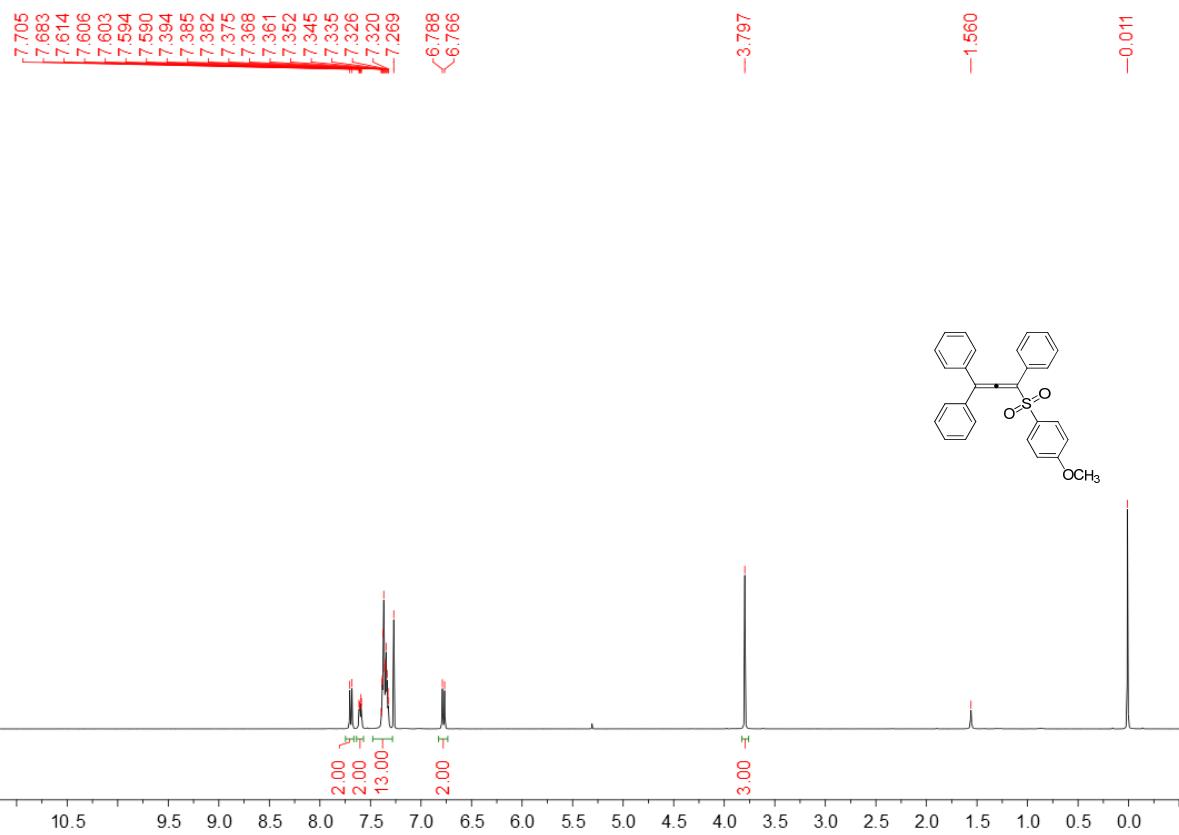
A single crystal **3a** with dimensions of 0.12 mm × 0.10 mm × 0.07 mm was mounted on a Siemens P1 diffractometer equipped with a graphite mono-chromated MoKa ( $\lambda = 0.71073 \text{ \AA}$ ) radiation at 298(2) K. A total of 10917 reflections were collected in the  $2.50 < \theta < 25.02^\circ$  range by using an  $\omega$  scan mode and 3945 were independent ( $R_{\text{int}} = 0.0739$ ), of which 1746 with  $I > 2\sigma(I)$  were observed. The calculations were performed with SHELXS-97 and SHELXS-97 programs and corrections for  $Lp$  factors and absorptions were applied. The structure was solved by direct methods. The non-hydrogen atoms were refined anisotropically, and the hydrogen atoms were determined by theoretical calculations. The final cycle of refinement gave  $R = 0.0496$  and  $wR = 0.0508$  ( $w = 1/[\sigma^2(F_0^2)+(0.0003P)^2+0.0000P]$ , where  $P = (F_0^2+2F_c^2)/3$ ).  $S = 0.925$ ,  $(\Delta/\sigma)_{\text{max}} = 0.000$ ,  $(\Delta\rho)_{\text{min}} = 0.162 \text{ e}/\text{\AA}^3$  and  $(\Delta\rho)_{\text{max}} = -0.181 \text{ e}/\text{\AA}^3$ .

The crystal of compound **3a** belongs to monoclinic, space group  $P2(1)/n$  with  $a = 10.5311(9)$ ,  $b = 14.0448(12)$ ,  $c = 15.9503(14) \text{ \AA}$ ,  $\beta = 108.442(2)^\circ$ ,  $V = 2238.0(3) \text{ \AA}^3$ ,  $Mr = 422.52$ ,  $Z = 4$ ,  $D_c = 1.254 \text{ g}/\text{cm}^3$ ,  $\mu(\text{MoK}\alpha) = 0.167 \text{ mm}^{-1}$ ,  $F(000) = 888$ , the final  $R = 0.0496$  and  $wR = 0.0508$ .

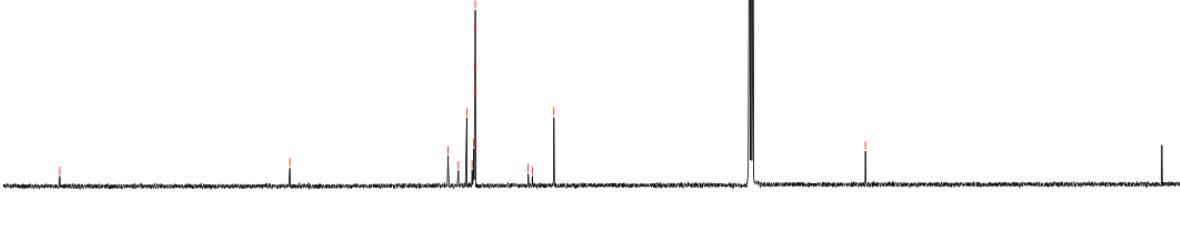
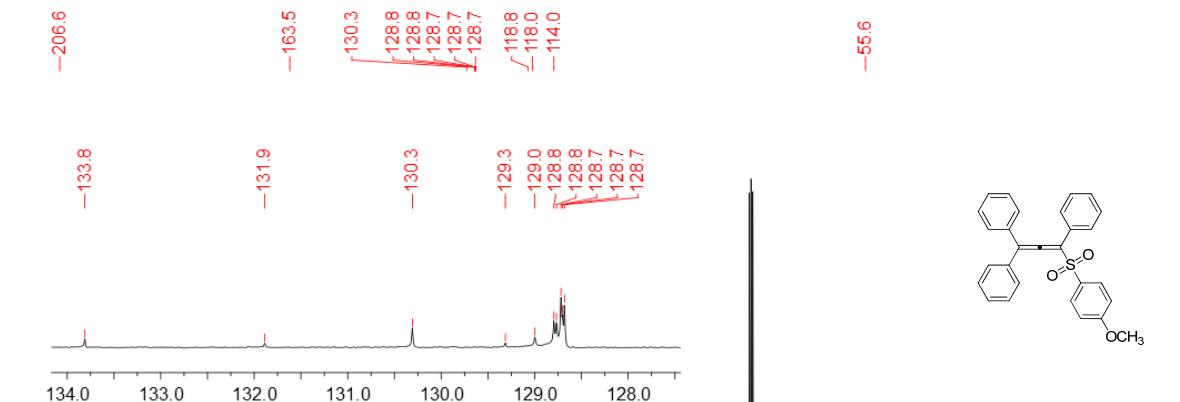
**Table 1.** Atomic Coordinates ( $\times 10^4$ ) and Thermal Parameters ( $\text{\AA}^2 \times 10^3$ )

atom	x	y	z	Ueq	atom	x	y	z	Ueq
O(1)	8070(2)	3680(1)	5176(1)	76(1)	C(14)	4788(3)	3601(3)	8515(2)	79(1)
O(2)	6941(2)	2188(1)	4524(1)	77(1)	C(15)	5043(3)	2858(2)	8027(2)	63(1)
S(1)	7224(1)	2893(1)	5219(1)	60(1)	C(16)	5706(3)	1119(2)	7157(2)	47(1)
C(1)	7965(3)	2313(2)	6264(2)	45(1)	C(17)	5766(2)	602(2)	7903(2)	58(1)
C(2)	7218(3)	2181(2)	6757(2)	48(1)	C(18)	5151(3)	-278(2)	7831(2)	67(1)
C(3)	6430(3)	2049(2)	7235(2)	47(1)	C(19)	4457(3)	-634(2)	7011(2)	68(1)
C(4)	9391(3)	2019(2)	6499(2)	48(1)	C(20)	4401(3)	-135(2)	6266(2)	66(1)
C(5)	10019(3)	1878(2)	5868(2)	65(1)	C(21)	5018(3)	739(2)	6341(2)	60(1)
C(6)	11316(3)	1534(2)	6105(2)	76(1)	C(22)	5706(3)	3316(2)	5310(2)	54(1)
C(7)	11982(3)	1327(2)	6980(3)	74(1)	C(23)	5712(3)	4083(2)	5854(2)	64(1)
C(8)	11384(3)	1486(2)	7615(2)	72(1)	C(24)	4535(4)	4356(2)	5988(2)	76(1)
C(9)	10090(3)	1829(2)	7378(2)	62(1)	C(25)	3340(4)	3890(2)	5578(2)	71(1)
C(10)	6224(3)	2809(2)	7820(2)	48(1)	C(26)	3362(3)	3148(2)	5013(2)	73(1)
C(11)	7144(3)	3528(2)	8115(2)	61(1)	C(27)	4534(3)	2859(2)	4883(2)	66(1)
C(12)	6900(4)	4272(2)	8598(2)	80(1)	C(28)	2076(3)	4168(2)	5761(2)	102(1)
C(13)	5720(4)	4315(2)	8795(2)	87(1)					

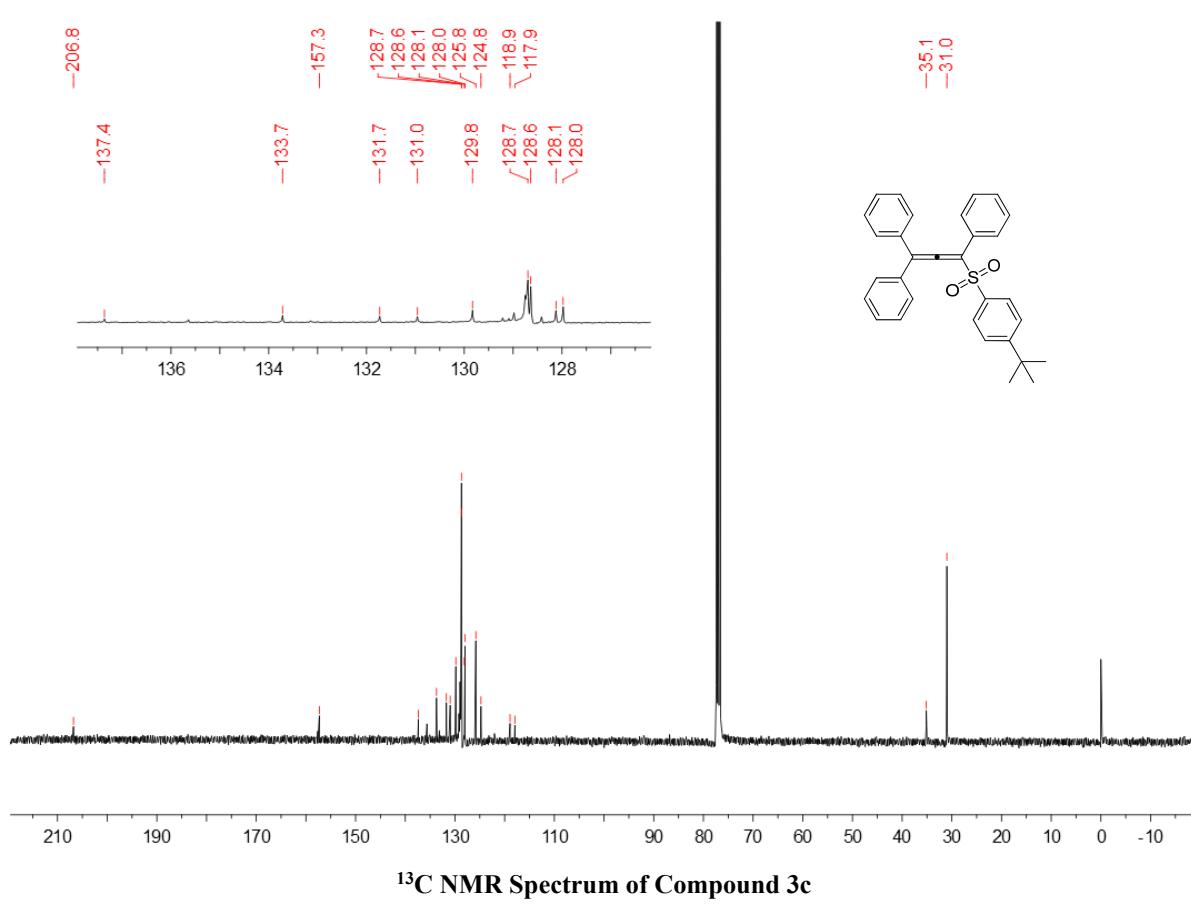
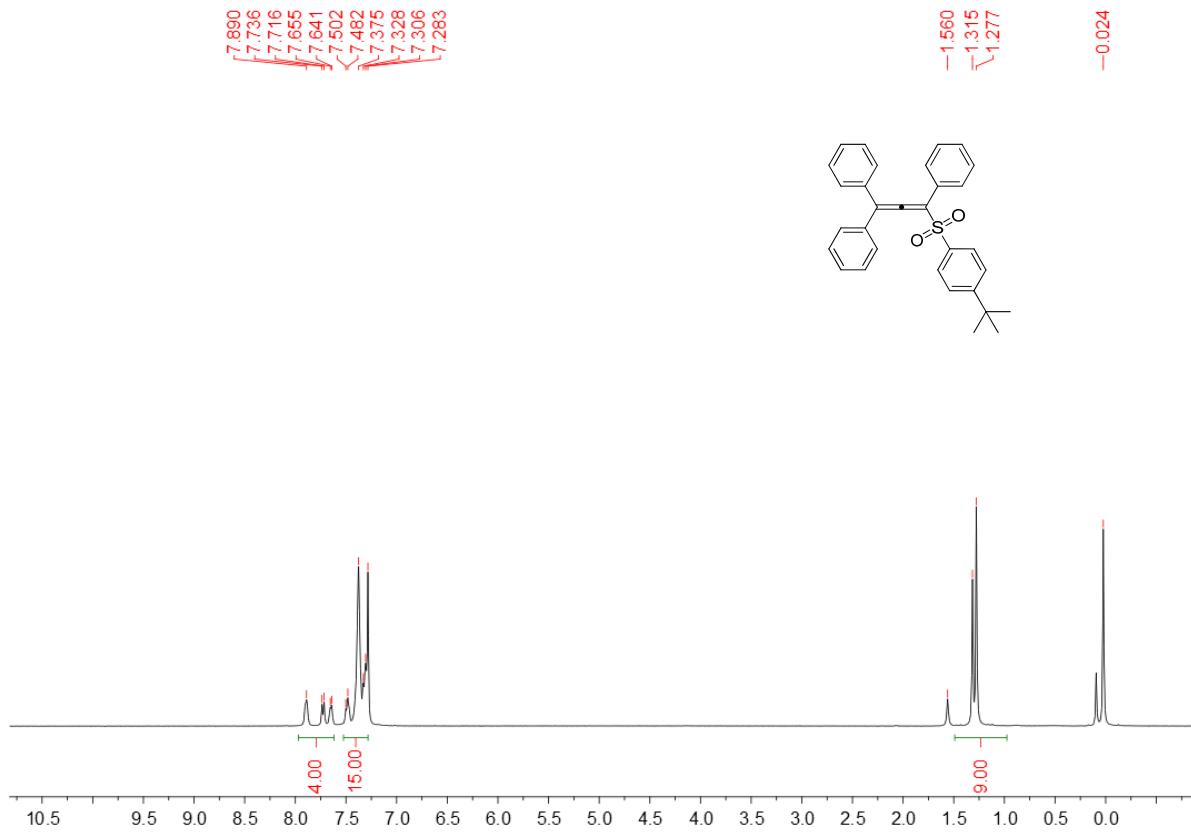


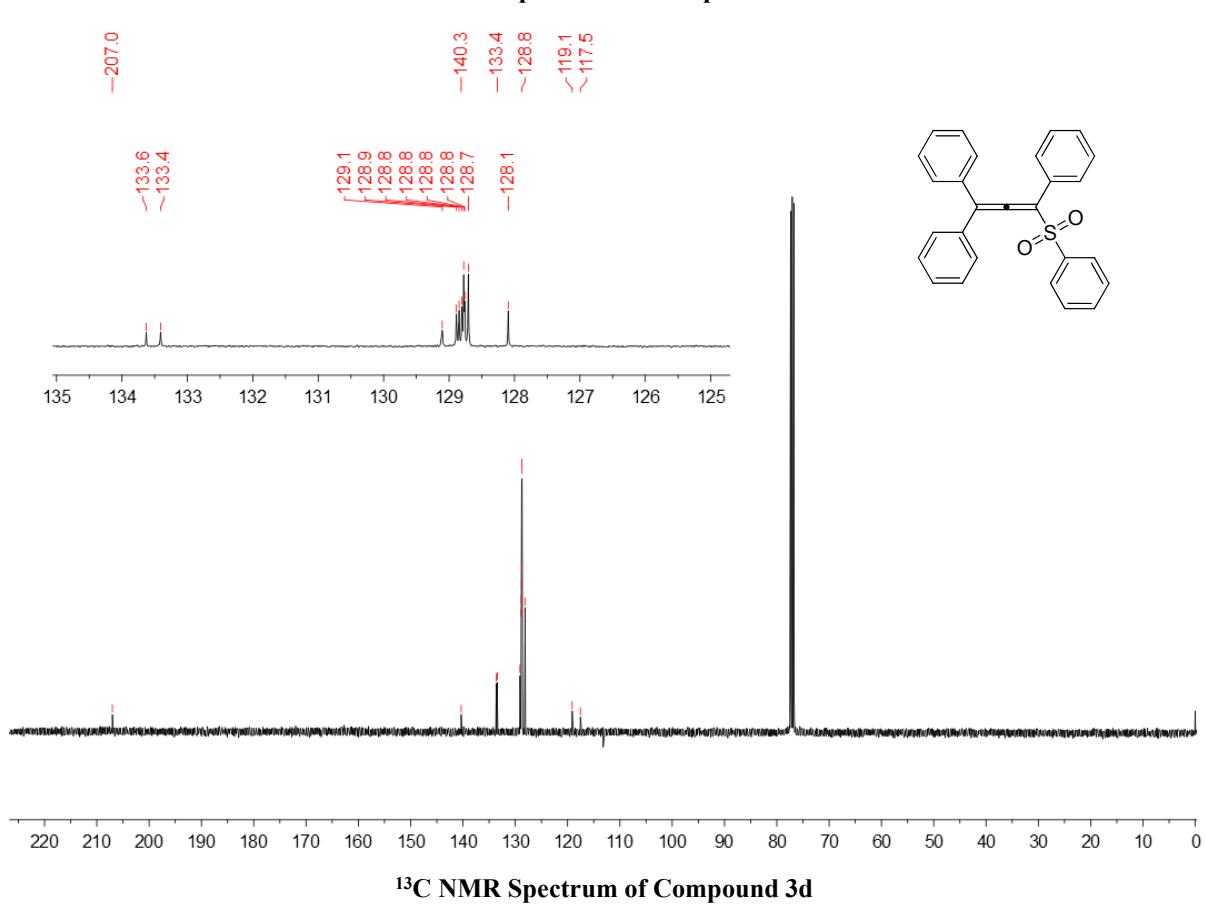
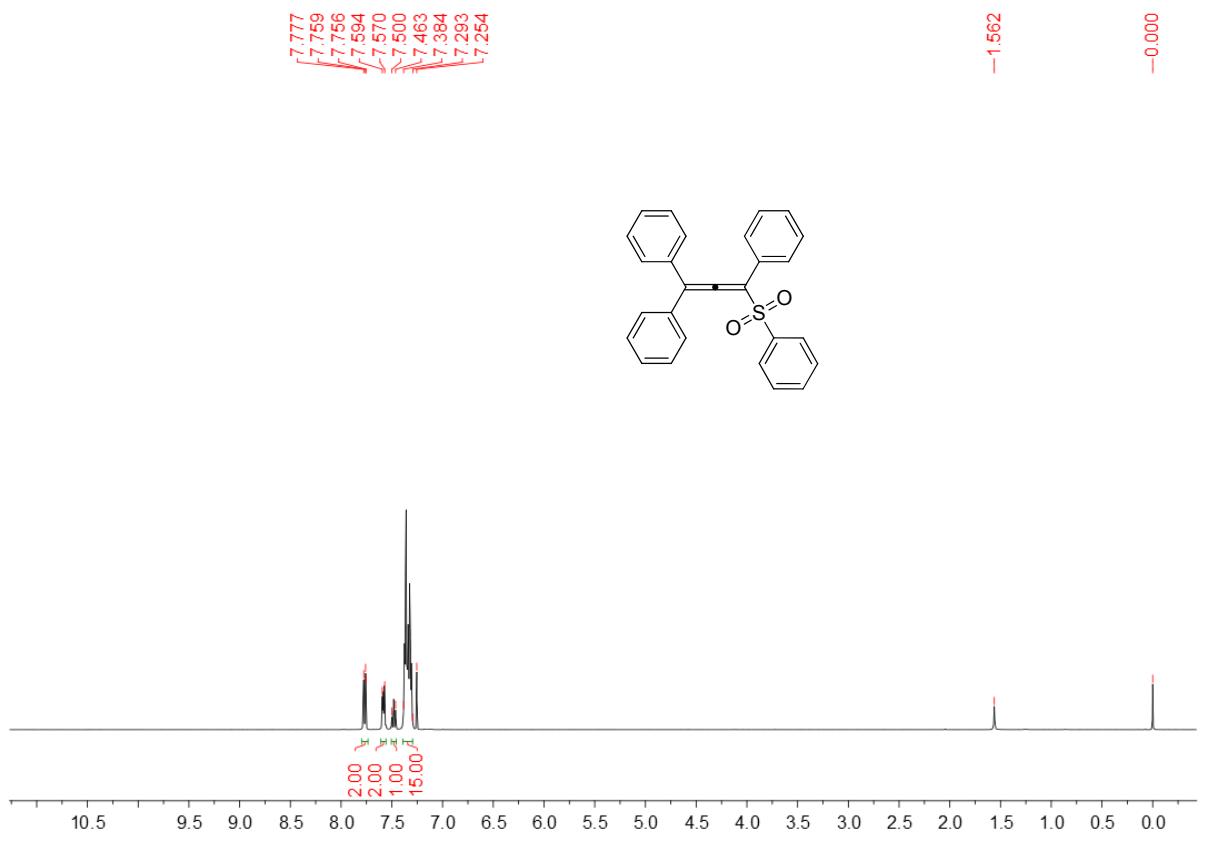


<sup>1</sup>H NMR Spectrum of Compound 3b

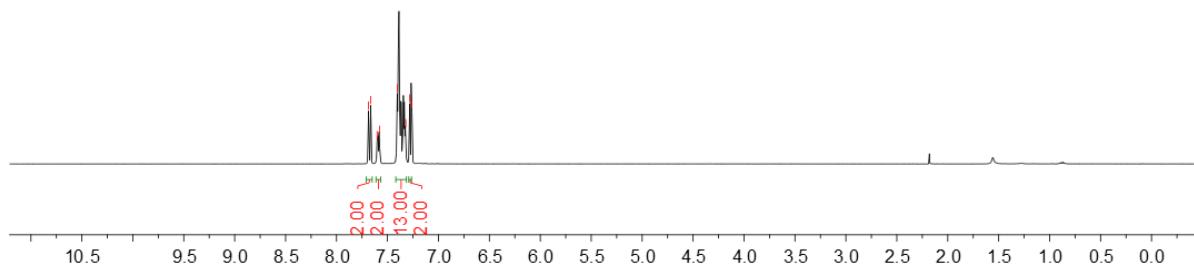
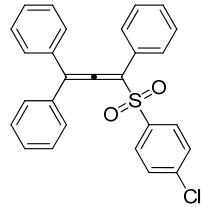


<sup>13</sup>C NMR Spectrum of Compound 3b





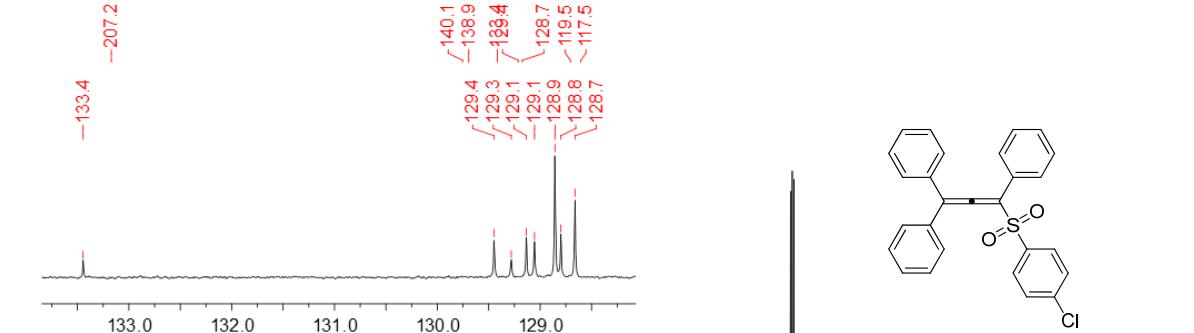
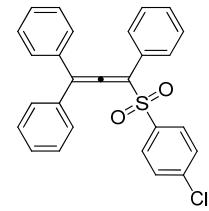
7.686  
7.664  
7.602  
7.578  
7.404  
7.320  
7.282  
7.260



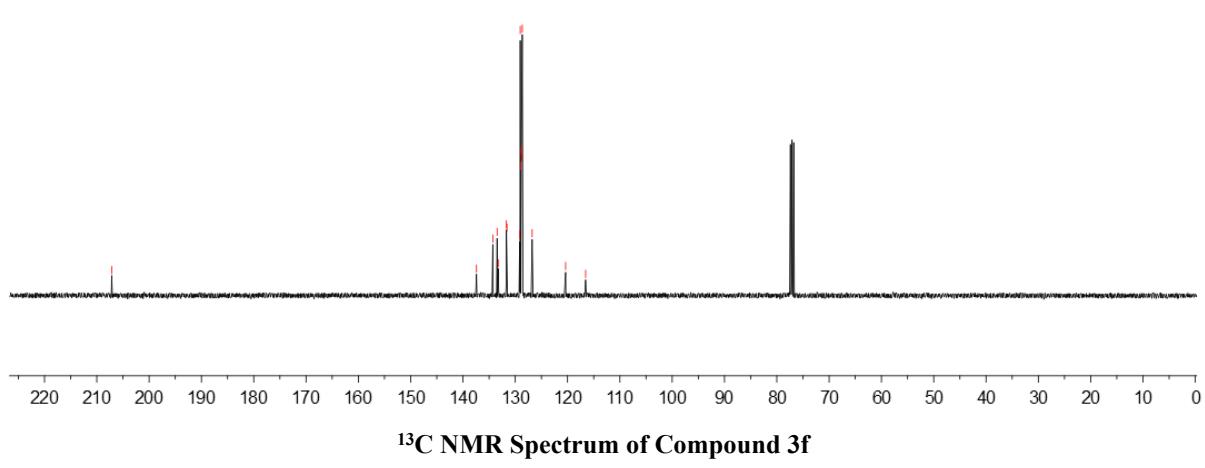
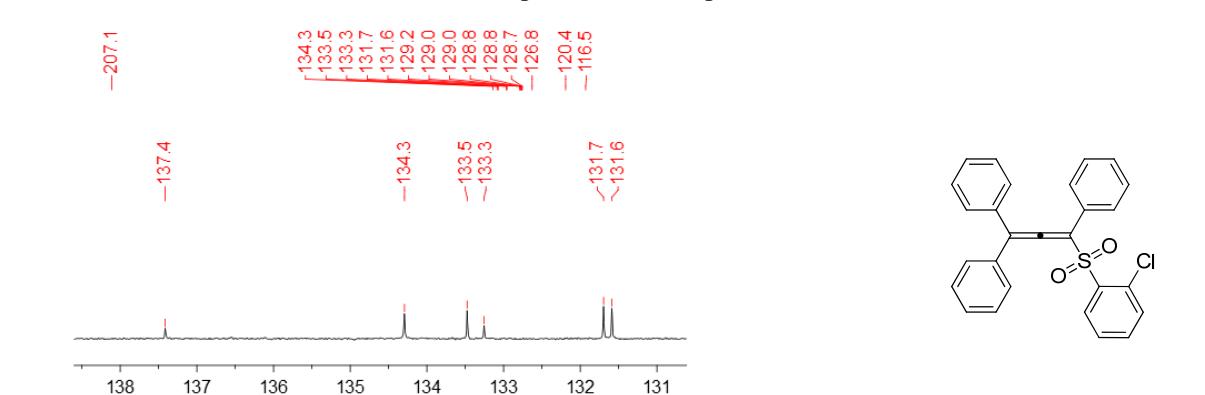
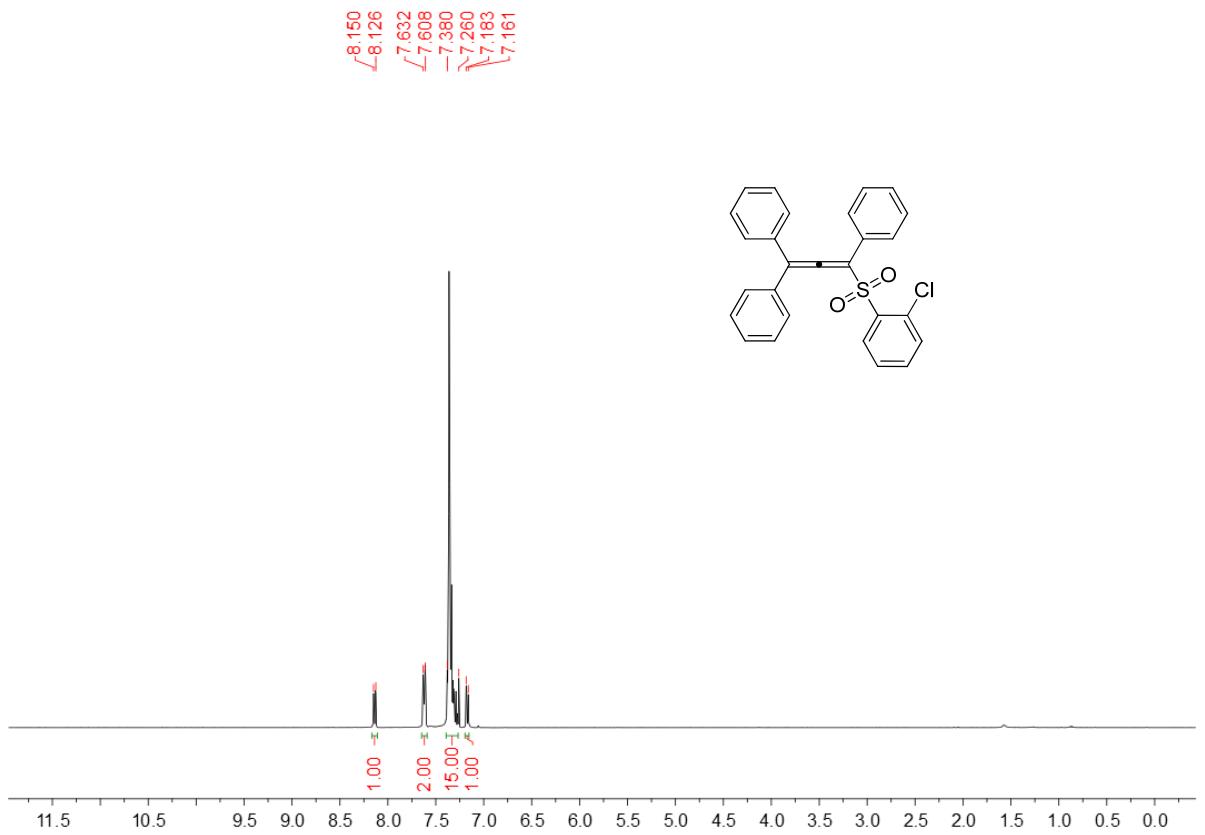
$^1\text{H}$  NMR Spectrum of Compound 3e

-133.4  
-207.2

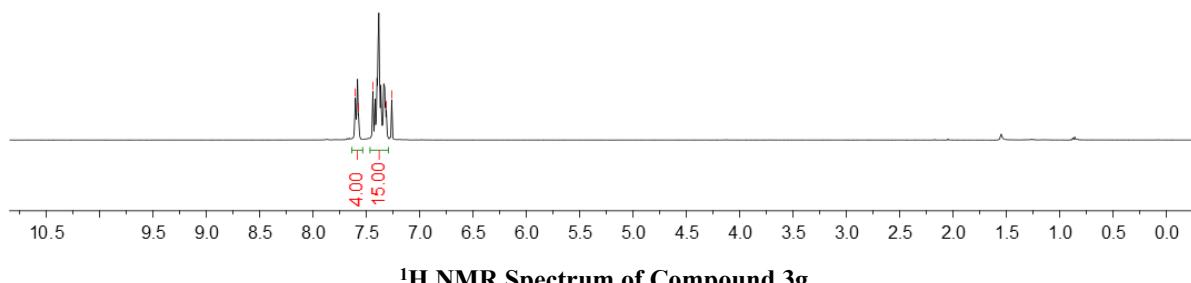
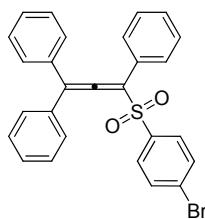
140.1  
138.9  
129.4  
129.3  
129.1  
129.1  
128.7  
128.9  
128.8  
128.7  
119.5  
117.5



$^{13}\text{C}$  NMR Spectrum of Compound 3e

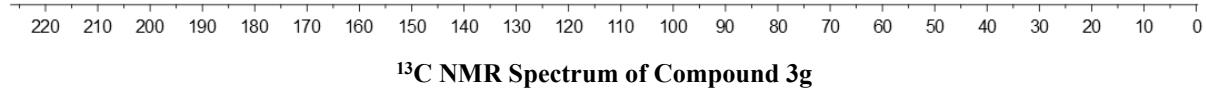
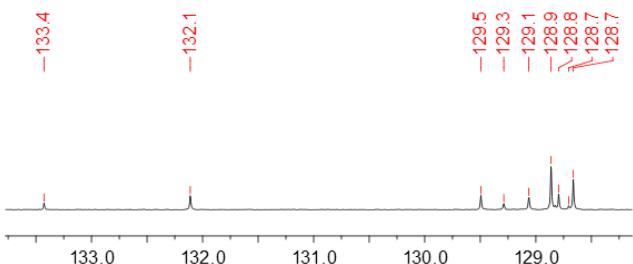
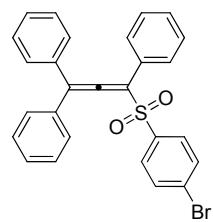


7.602  
7.572  
7.437  
7.311  
7.260

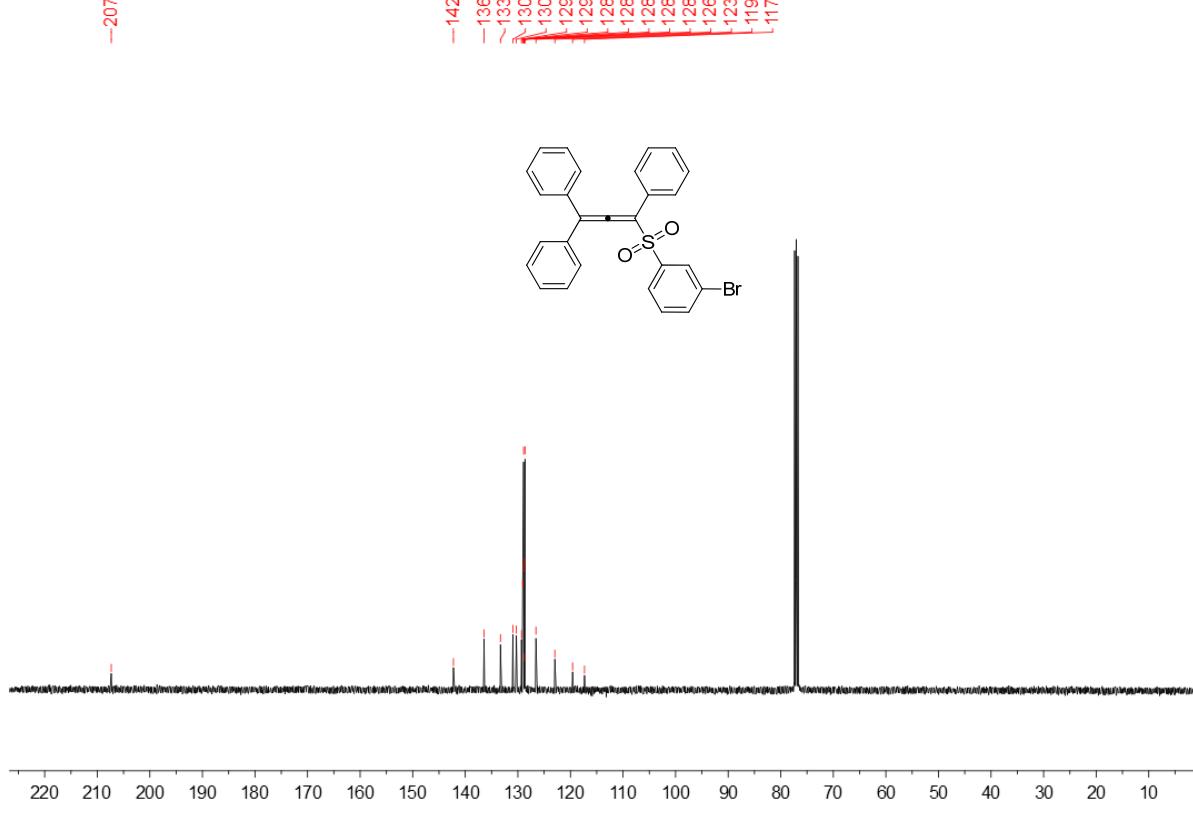
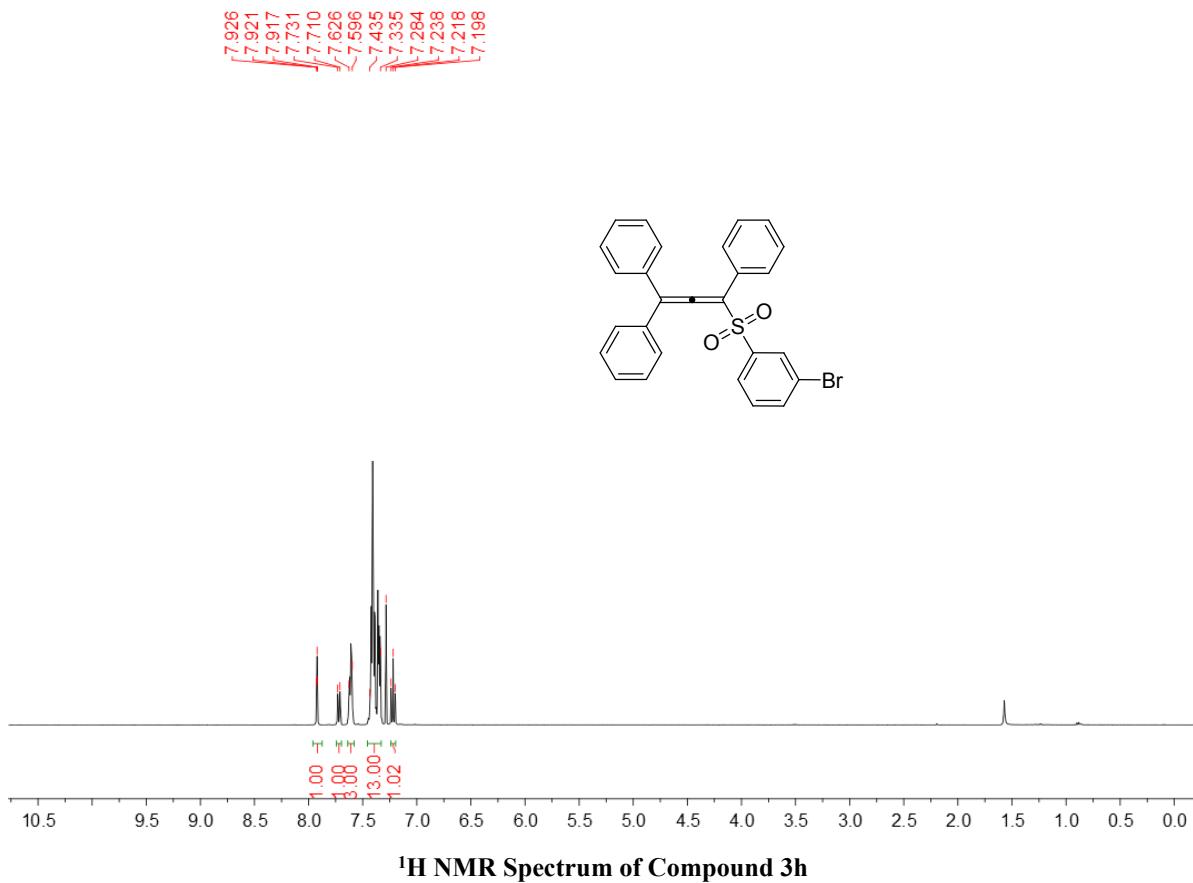


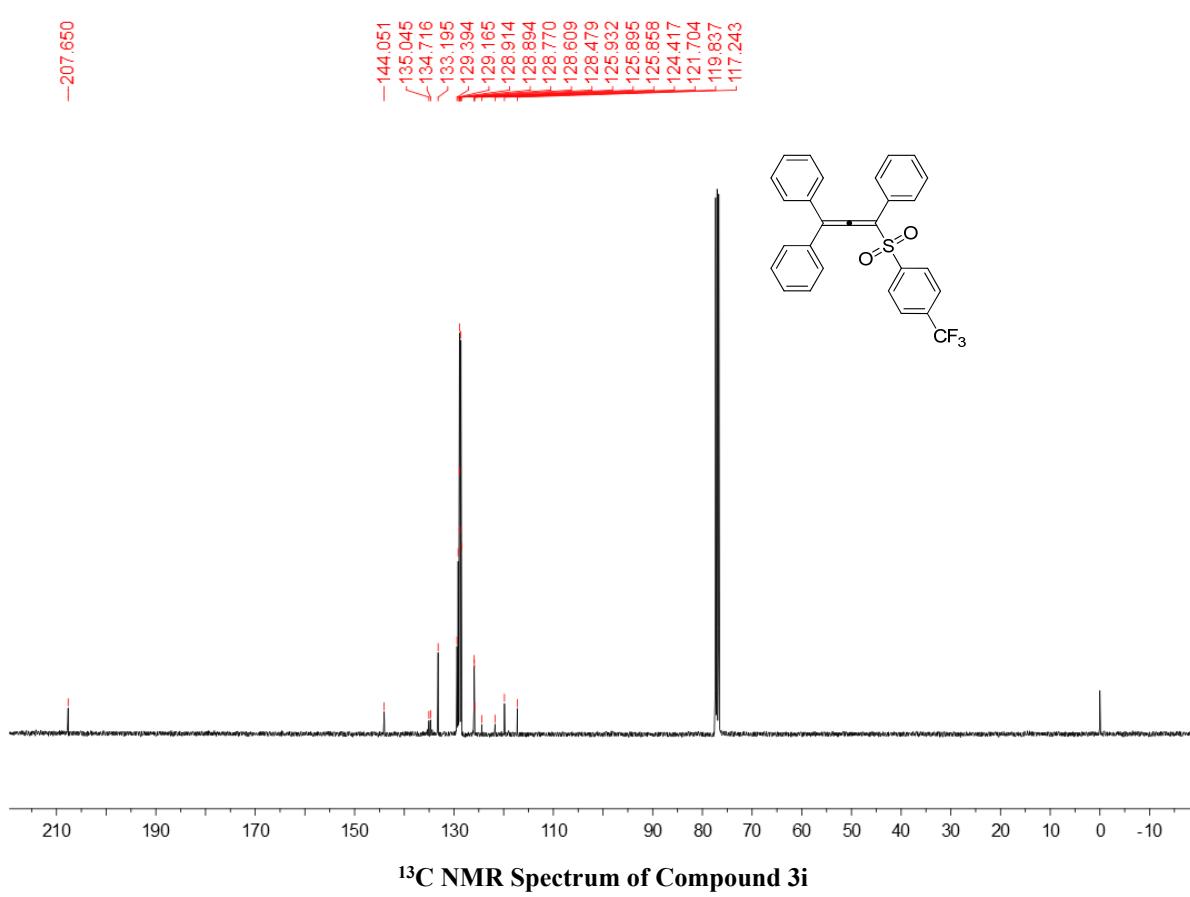
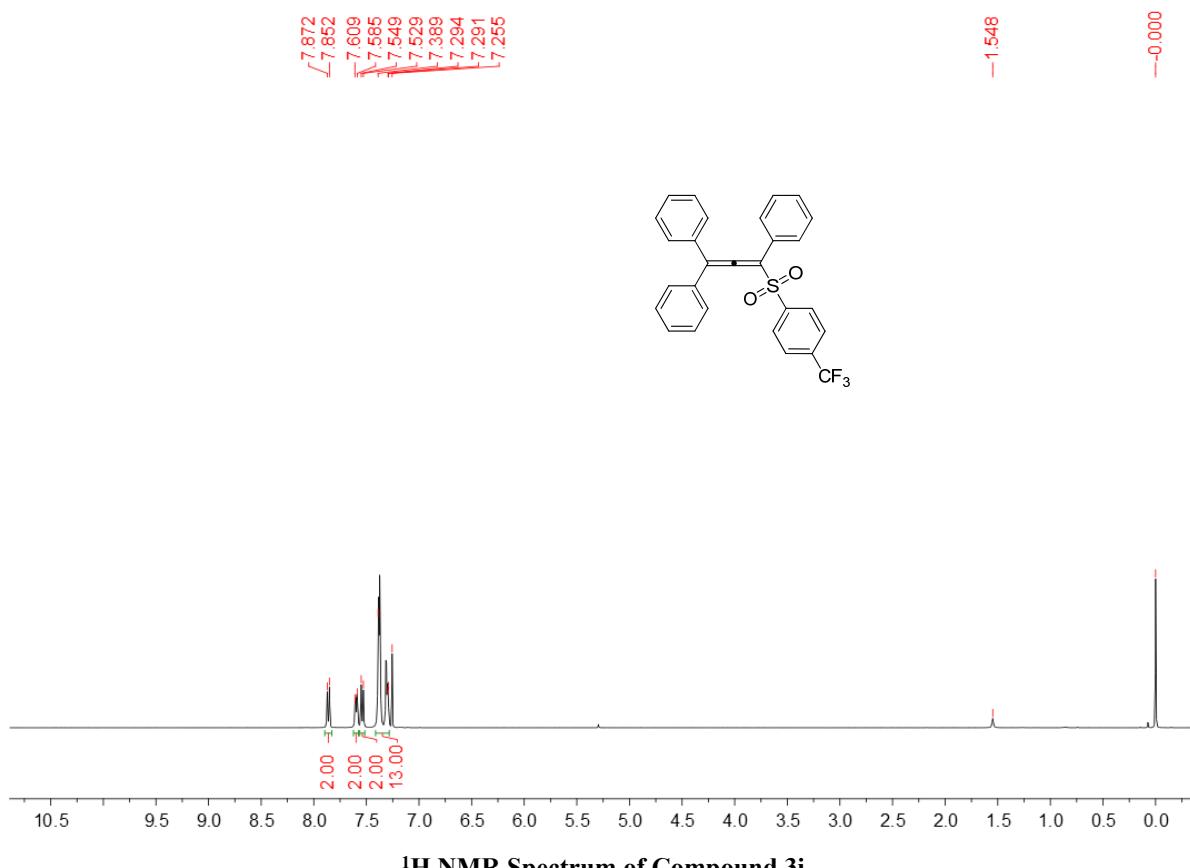
-133.4  
-207.3

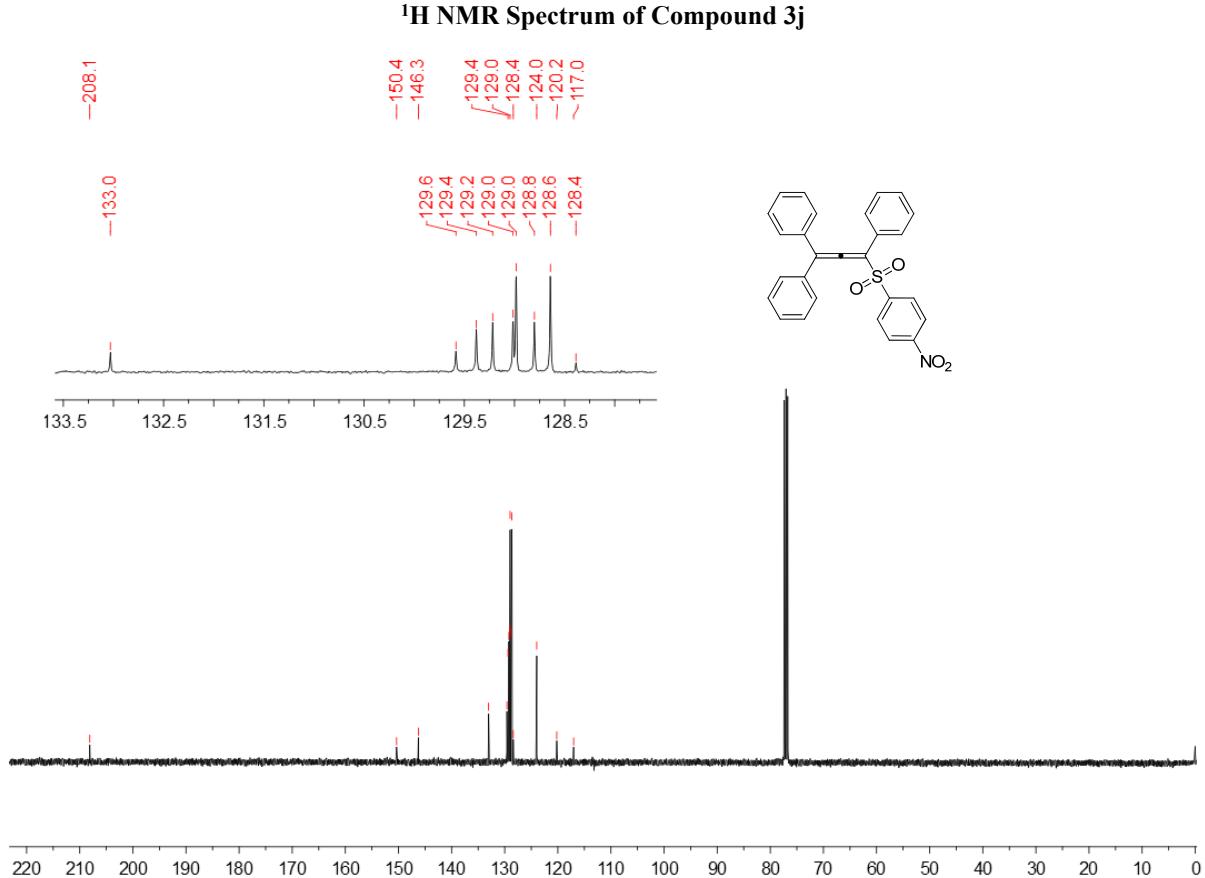
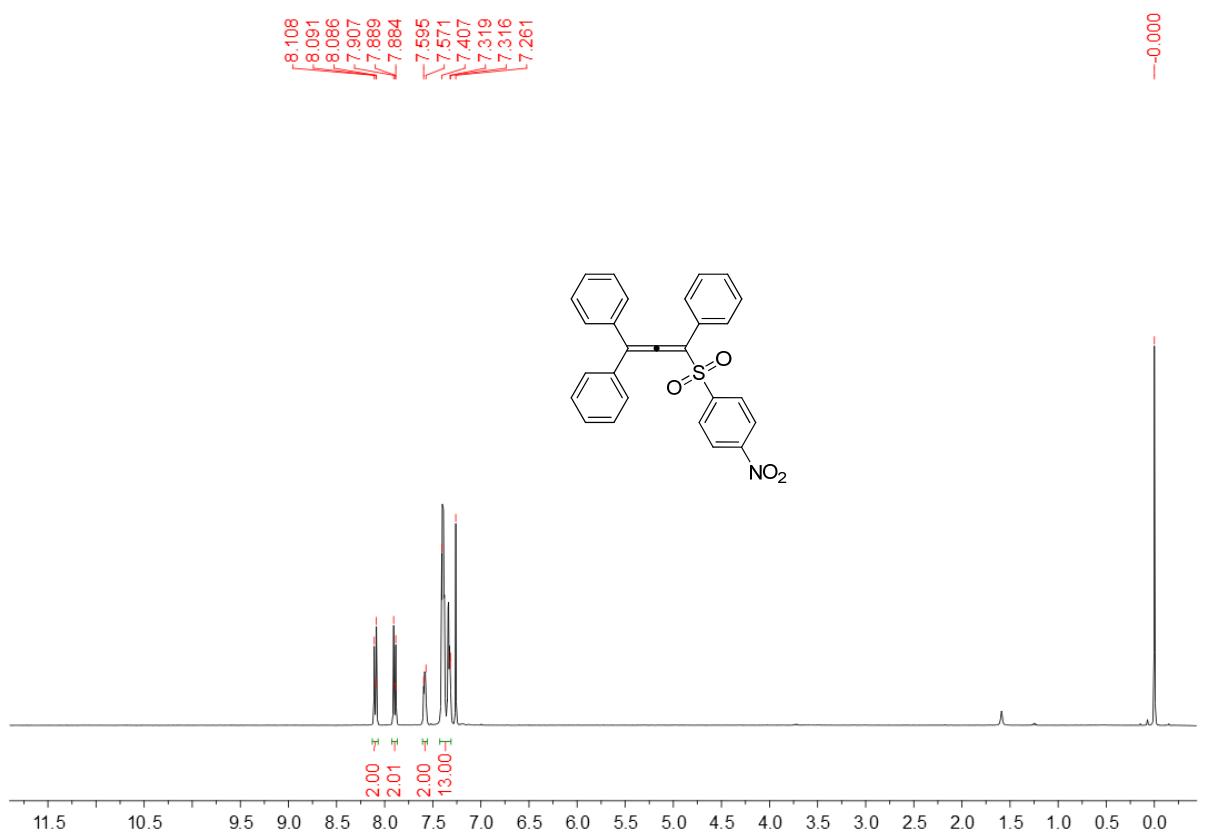
-139.5  
-129.5  
-128.9  
-128.9  
-128.9  
-128.9  
-128.7  
-128.7

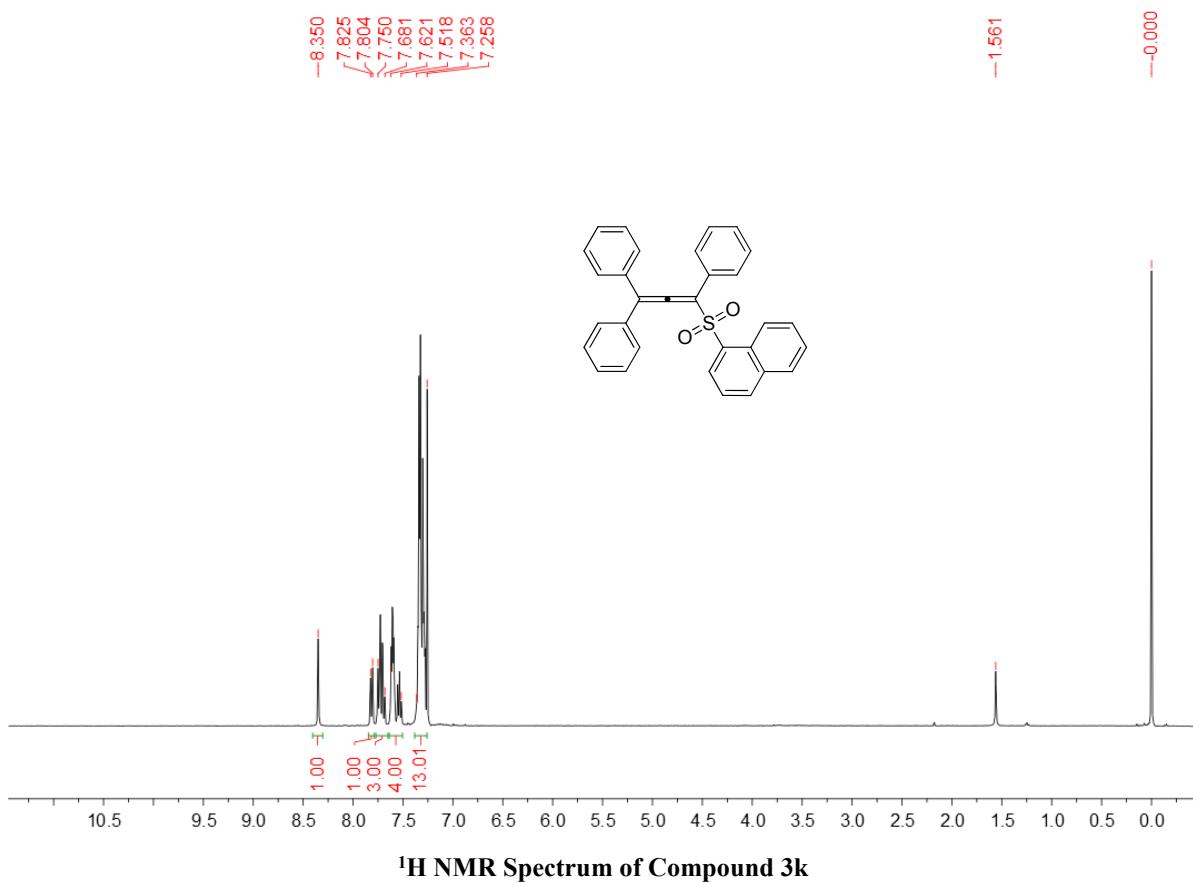


13C NMR Spectrum of Compound 3g

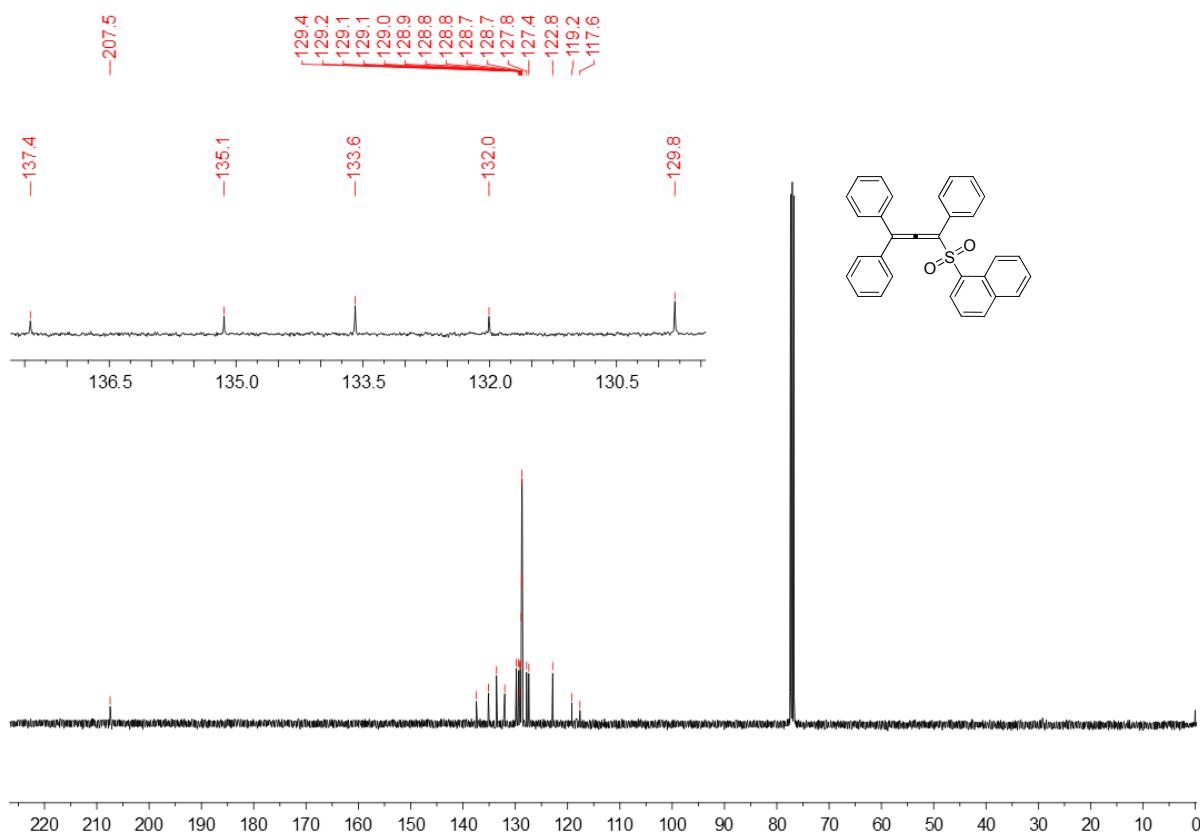




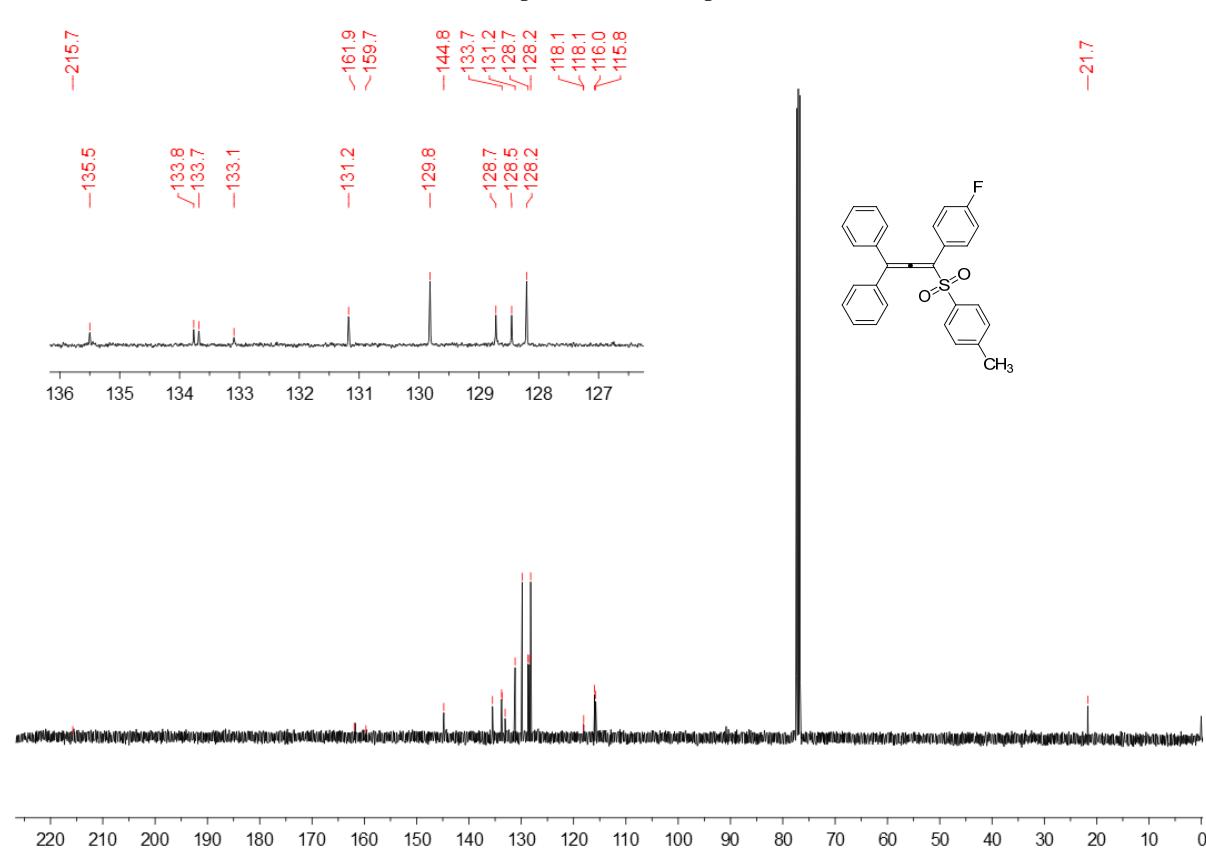
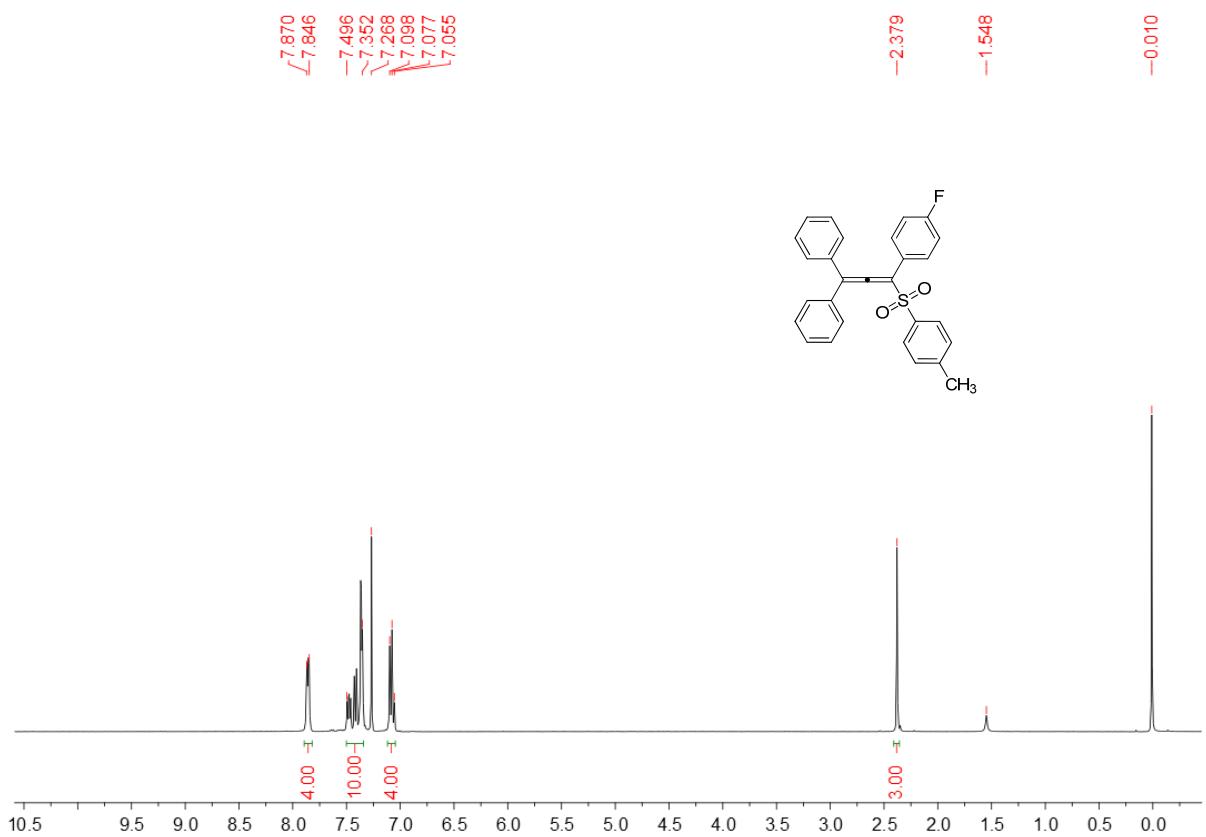


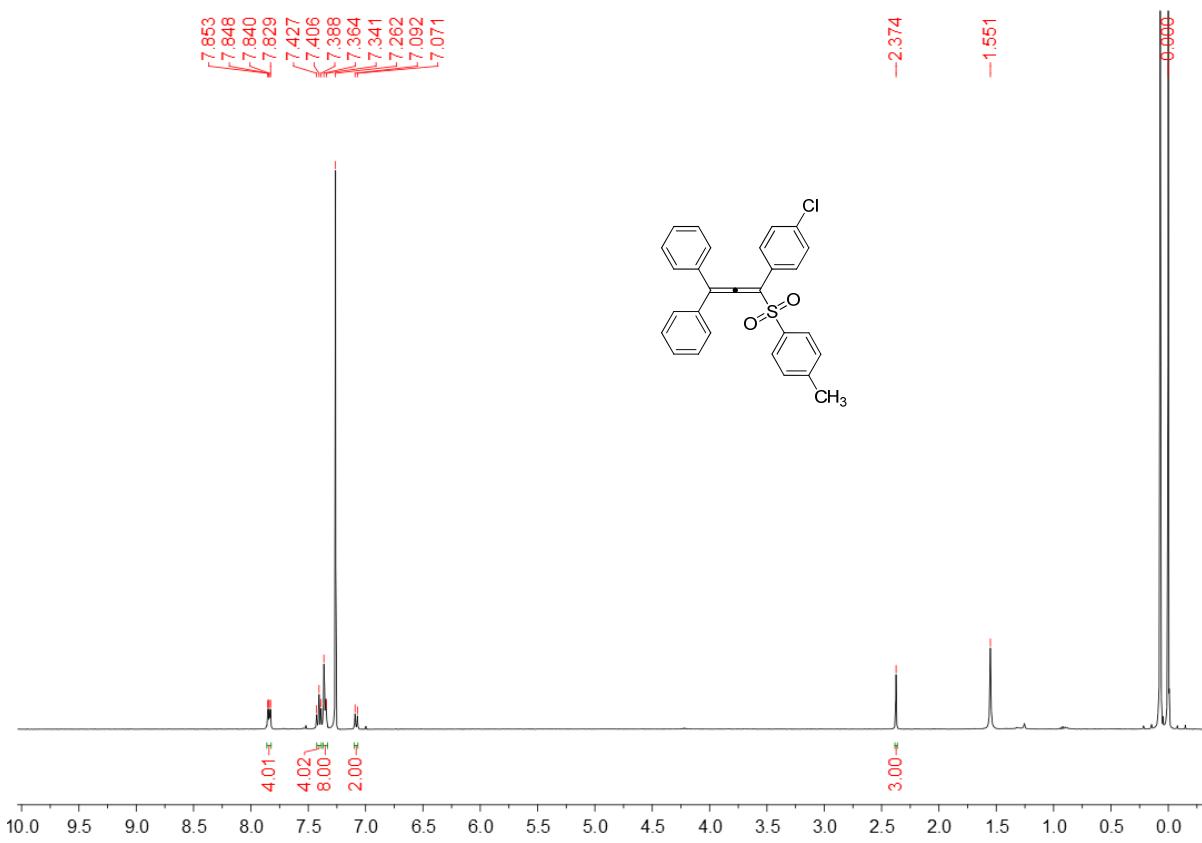


<sup>1</sup>H NMR Spectrum of Compound 3k

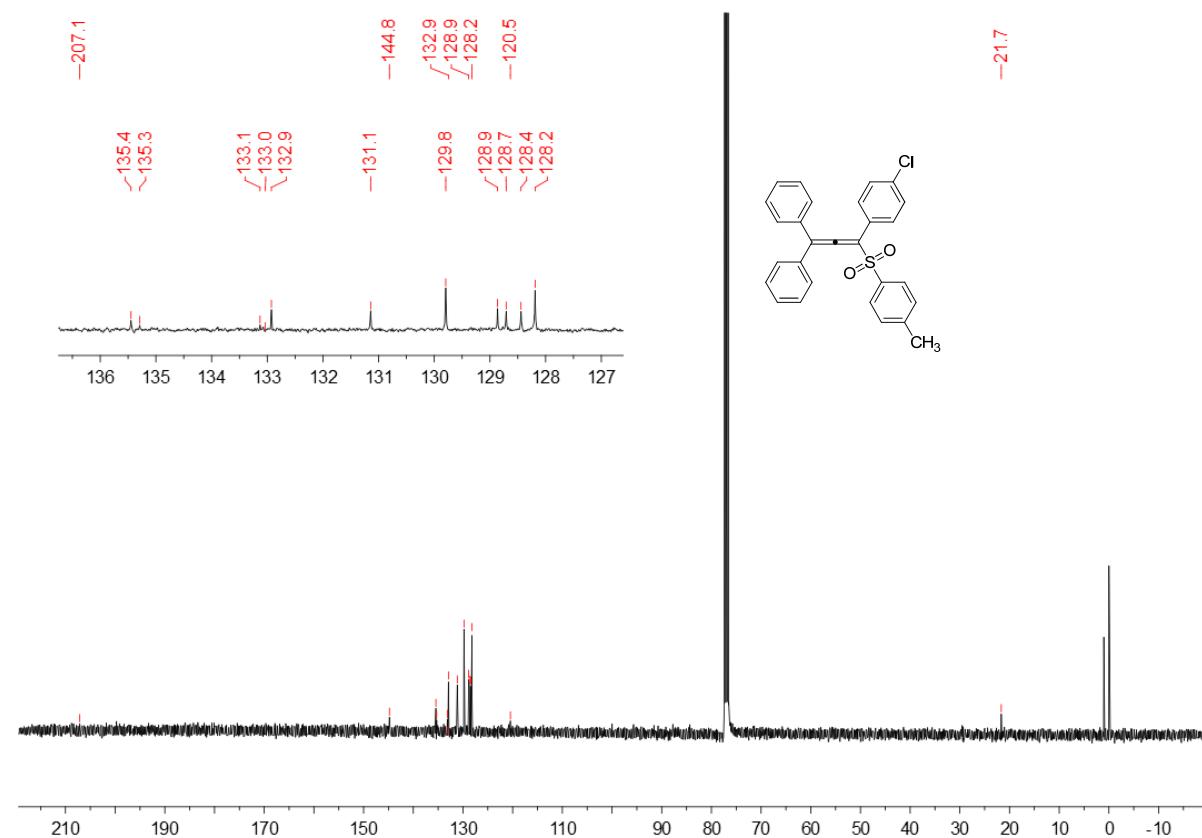


<sup>13</sup>C NMR Spectrum of Compound 3k





<sup>1</sup>H NMR Spectrum of Compound 3n



<sup>13</sup>C NMR Spectrum of Compound 3n

