Supporting information

Copper-Catalyzed Sulfenylation, Sulfonylation, and Selenylation of 2,3-Allenoic Acids with Disulfides or Diselenides

Ya-Xun Xin,[†] Shen Pan,[†] Yangen Huang,[†] Xiu-Hua Xu,*[‡] and Feng-Ling Qing[†,‡]*

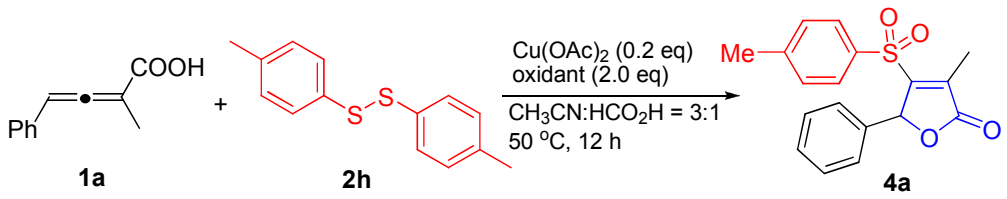
[†] College of Chemistry, Chemical Engineering and Biotechnology, Donghua University, 2999 North Renmin Lu, Shanghai 201620, China

[‡] Key Laboratory of Organofluorine Chemistry, Center for Excellence in Molecular Synthesis, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Lu, Shanghai 200032, China

E-mail: hyg@dhu.edu.cn, xuxiuhua@sioc.ac.cn

Table of Contents

1. Optimization of Reaction Conditions for Sulfonylation of 2,3-Allenoic Acid 1a[a]

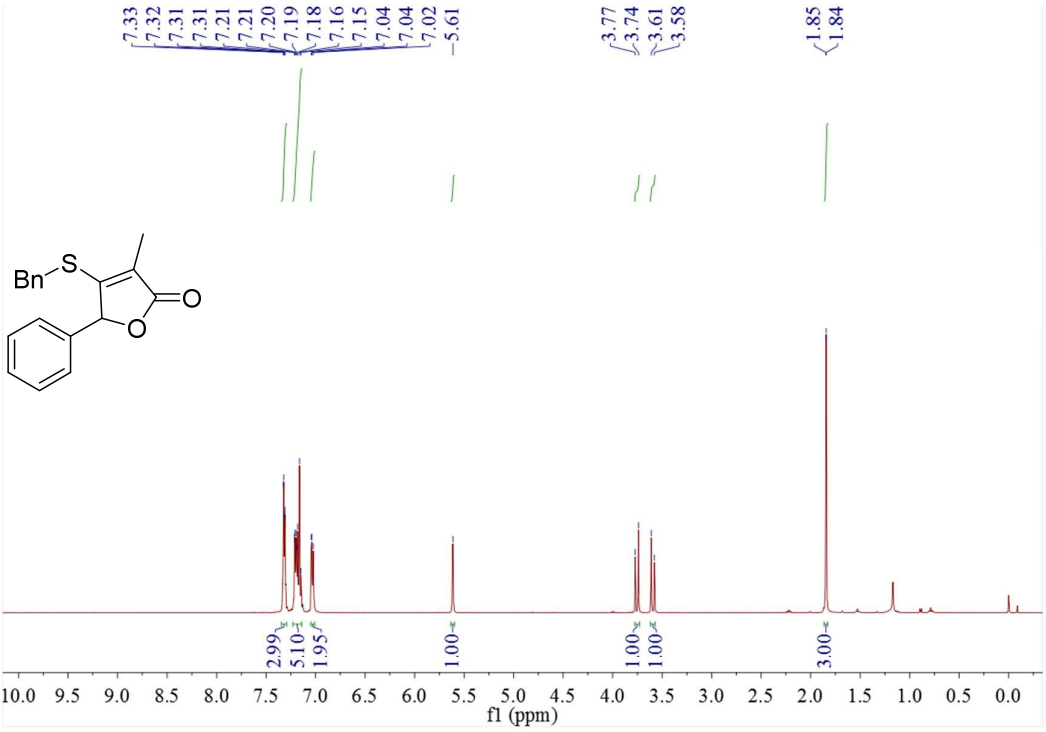


entry	oxidant	yield (%)[b]
1	$(NH_4)_2S_2O_8$	40
2	$(NH_4)_2S_2O_8$ (5.0 equiv)	41
3	$Na_2S_2O_8$	19
4	H_2O_2	5
5	*m*-CPBA	52
6	*m*-CPBA (5.0 equiv)	48
7	$(NH_4)_2S_2O_8$ + *m*-CPBA (2.0 equiv)	46
8	$(NH_4)_2S_2O_8$ + *m*-CPBA (2.0 equiv)[c]	77
9	$(NH_4)_2S_2O_8$ + *m*-CPBA (3.0 equiv)[c]	84
10	$(NH_4)_2S_2O_8$ + *m*-CPBA (5.0 equiv)[c]	92

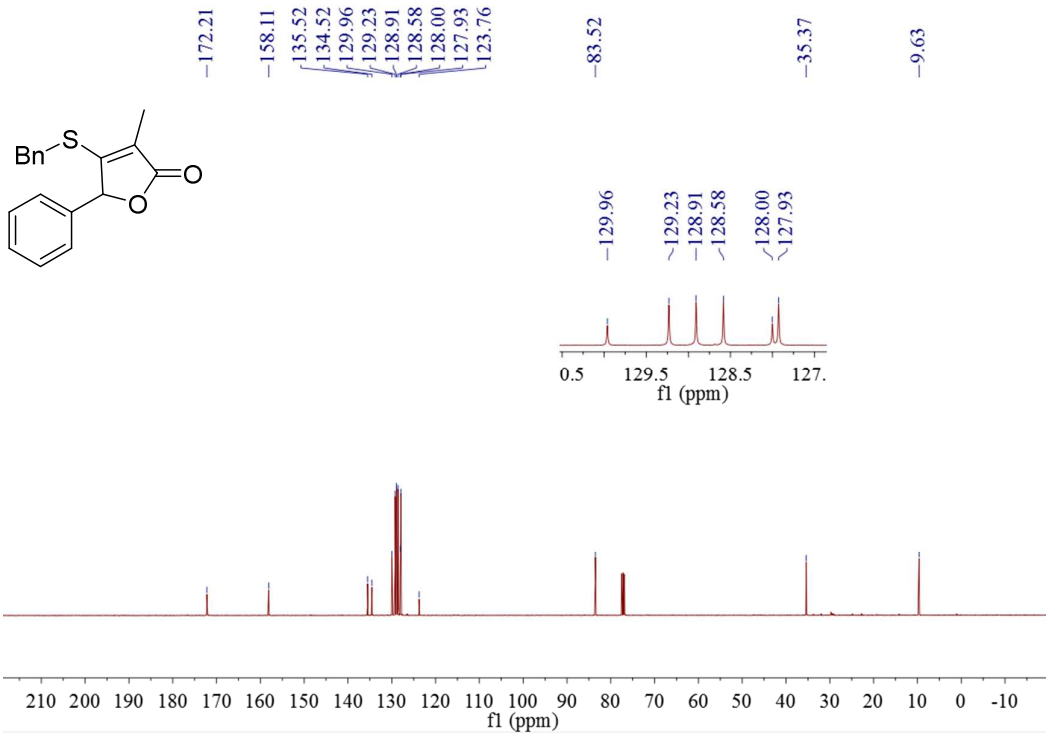
[a]Reaction conditions: **1a** (0.1 mmol), **2h** (0.2 mmol), $Cu(OAc)_2$ (0.02 mmol), oxidant (0.2 mmol), CH_3CN/HCO_2H (1.5 mL/0.5 mL), under N_2, 50 °C, 12 h. [b]Yields were determined by ^1H NMR spectroscopy using 1,3,5-trimethylphenol as an internal standard. [c]After 12 h at 50 °C, *m*-CPBA was added to the crude reaction mixture in CH_3CN (1.5 mL)/DCM (5.0 mL) and the reaction mixture was stirred at rt for 2 h.

2. Copies of ^{1}H, ^{19}F, and ^{13}C NMR Spectra for the Products

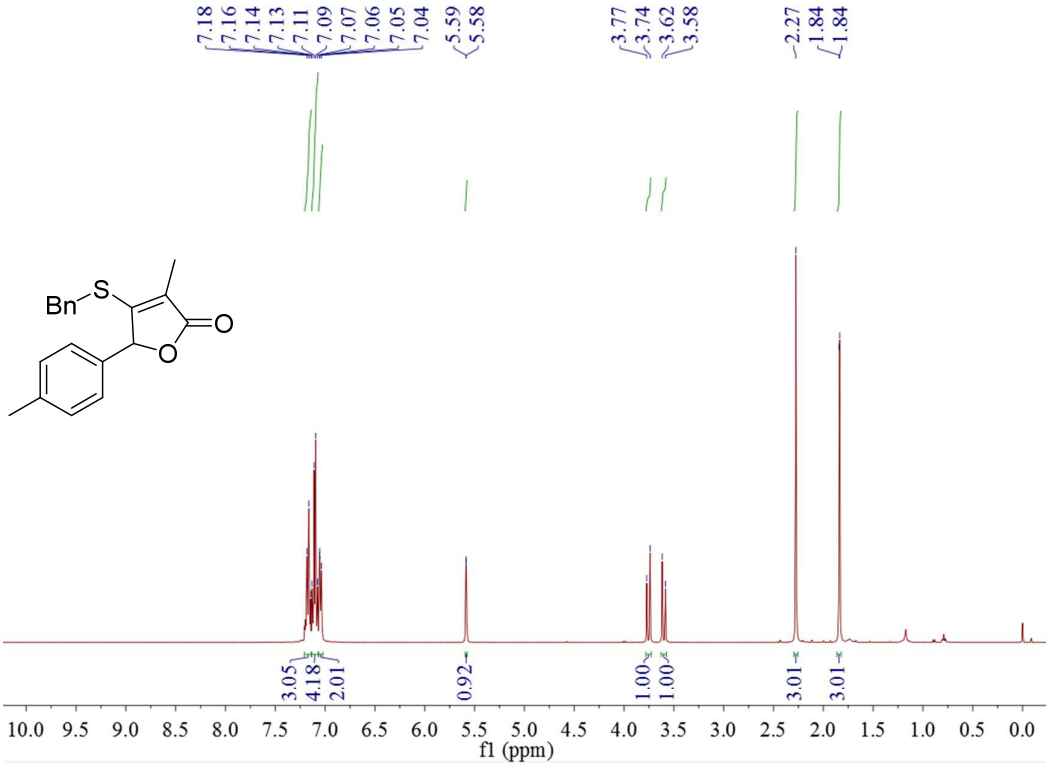
^{1}H NMR spectrum of **3a** in $CDCl_3$



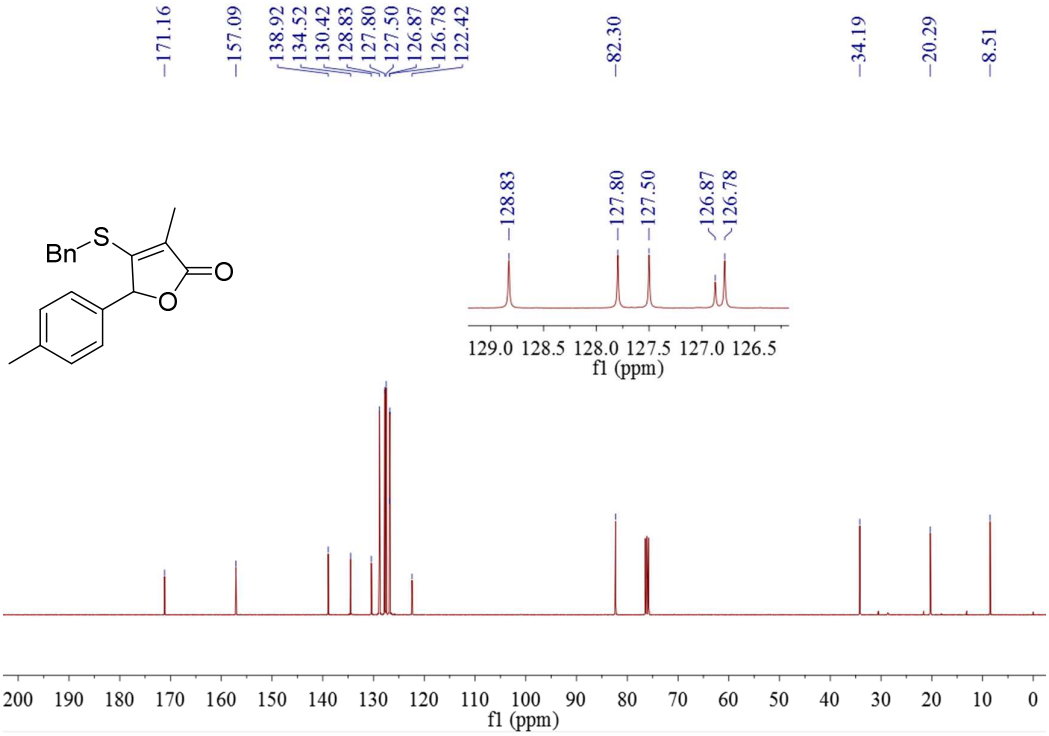
^{13}C NMR spectrum of **3a** in $CDCl_3$



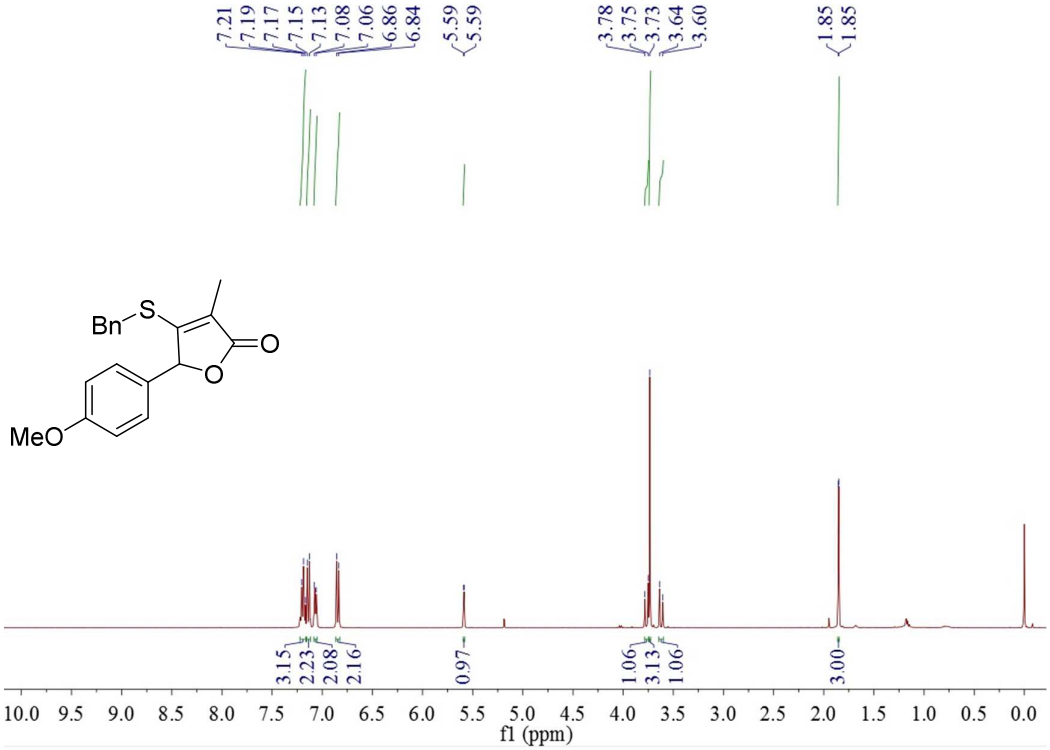
^{1}H NMR spectrum of **3b** in $CDCl_3$



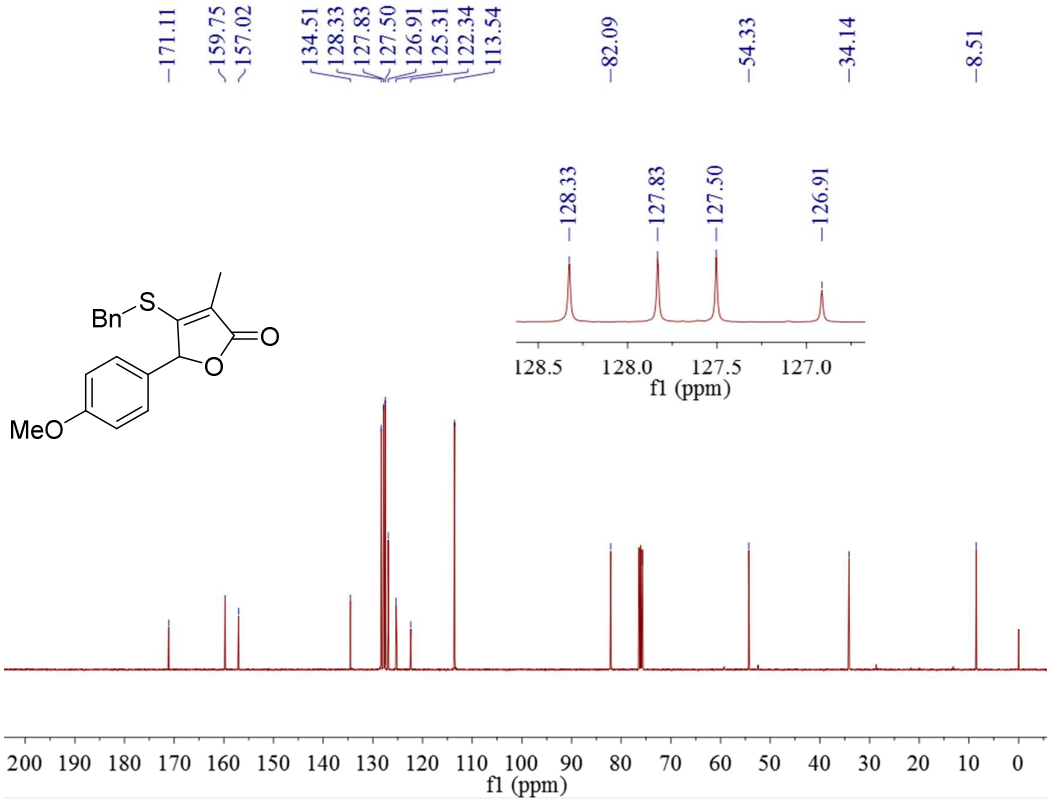
^{13}C NMR spectrum of **3b** in $CDCl_3$



^{1}H NMR spectrum of **3c** in $CDCl_3$



^{13}C NMR spectrum of **3c** in $CDCl_3$



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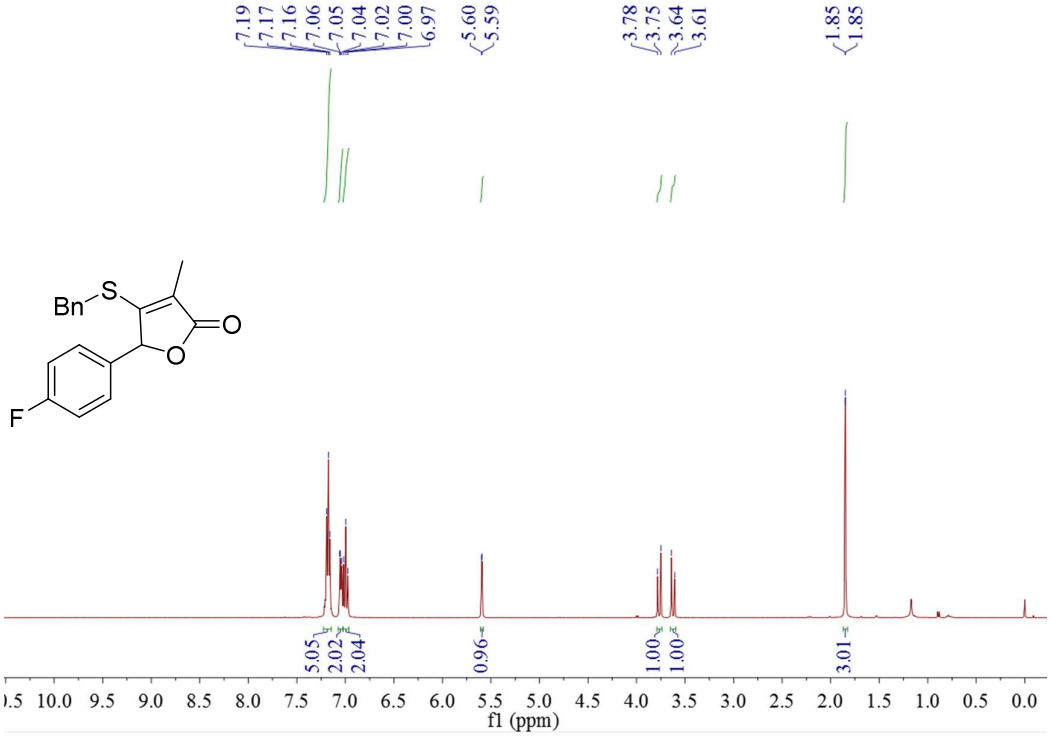

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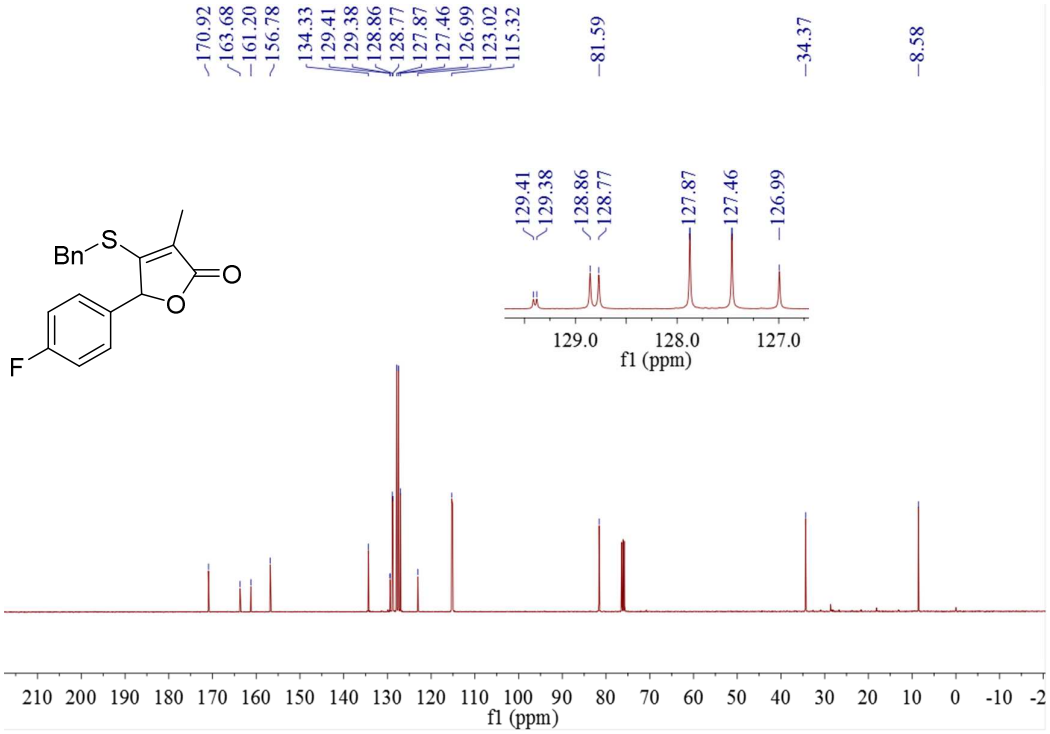

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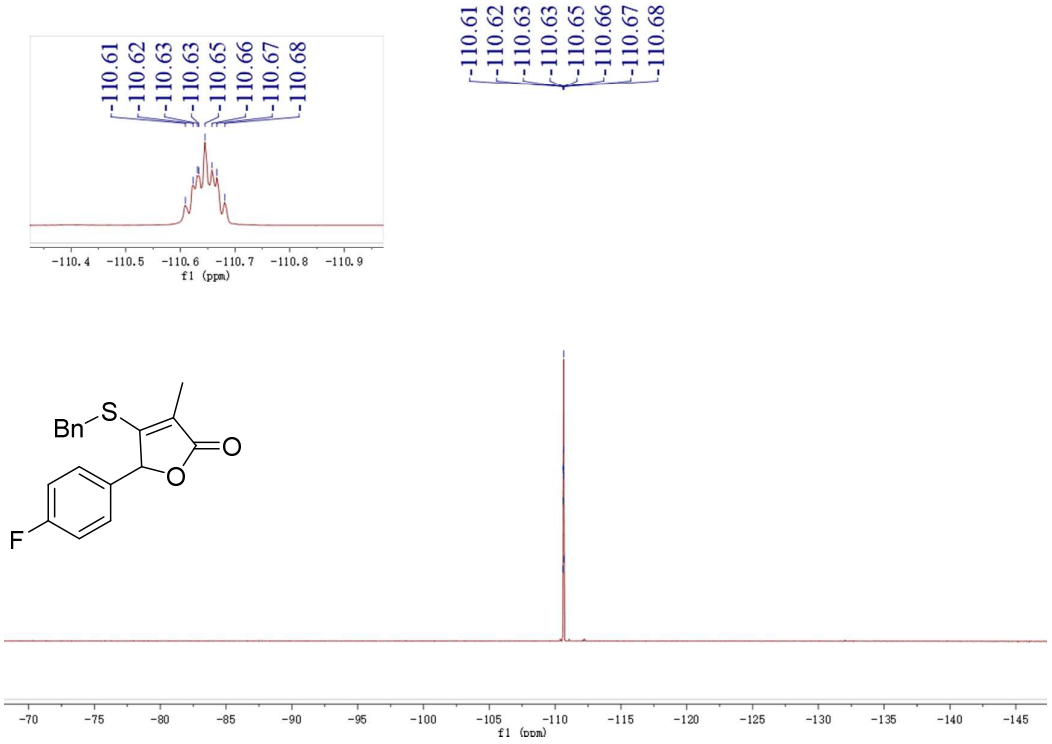

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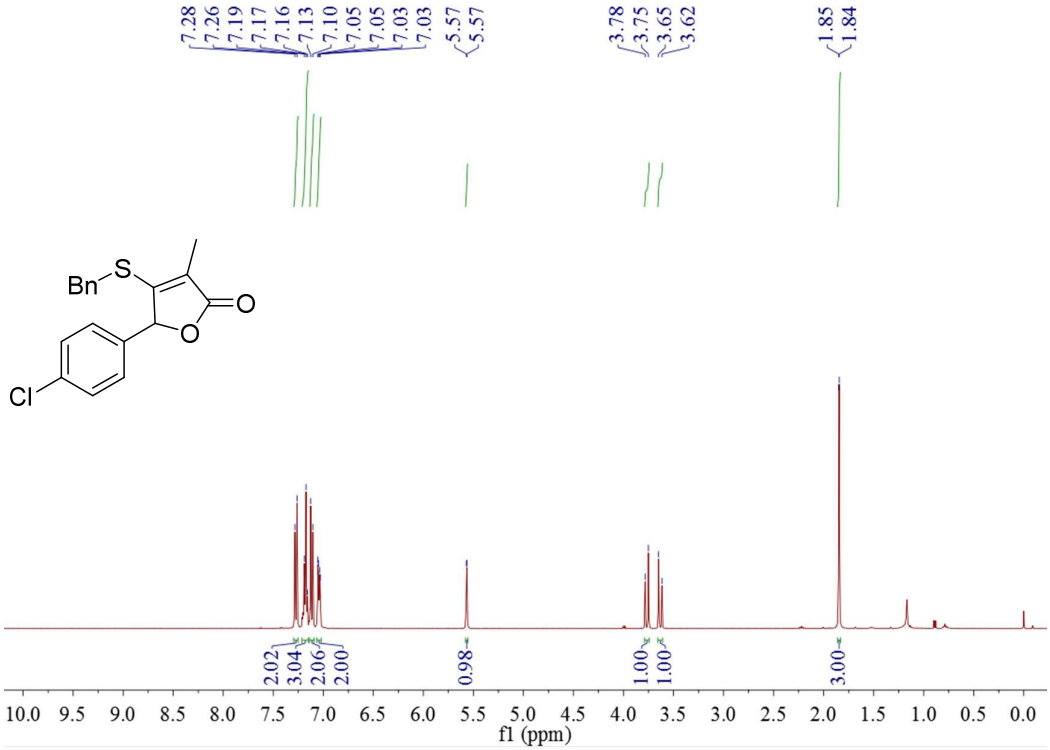
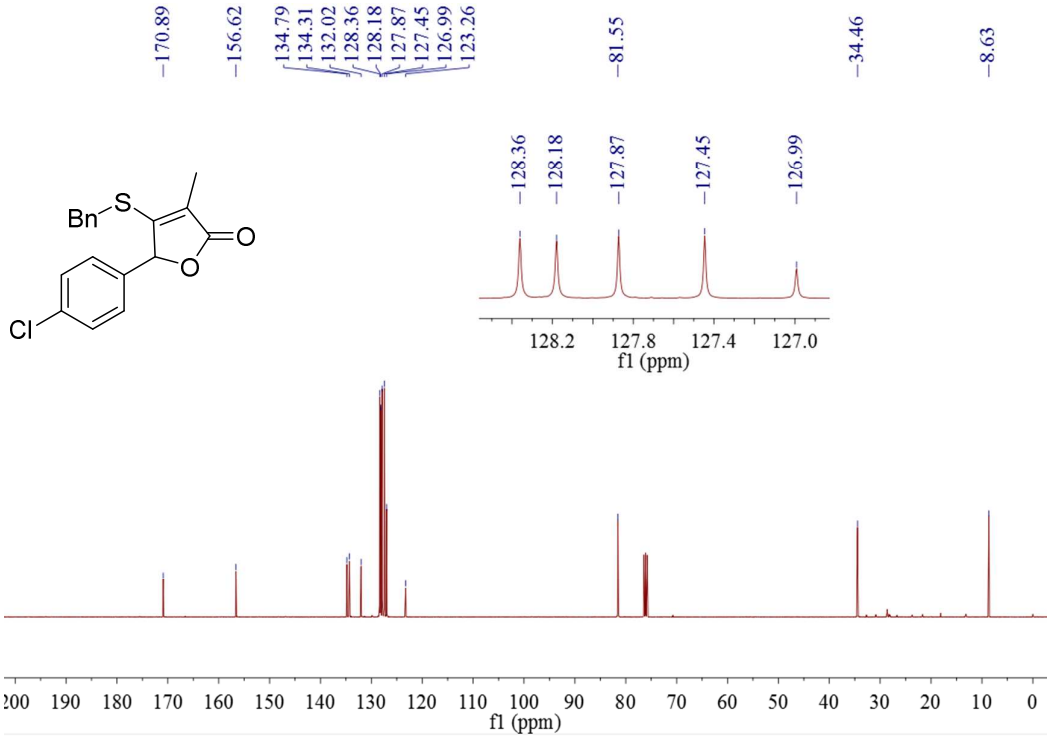
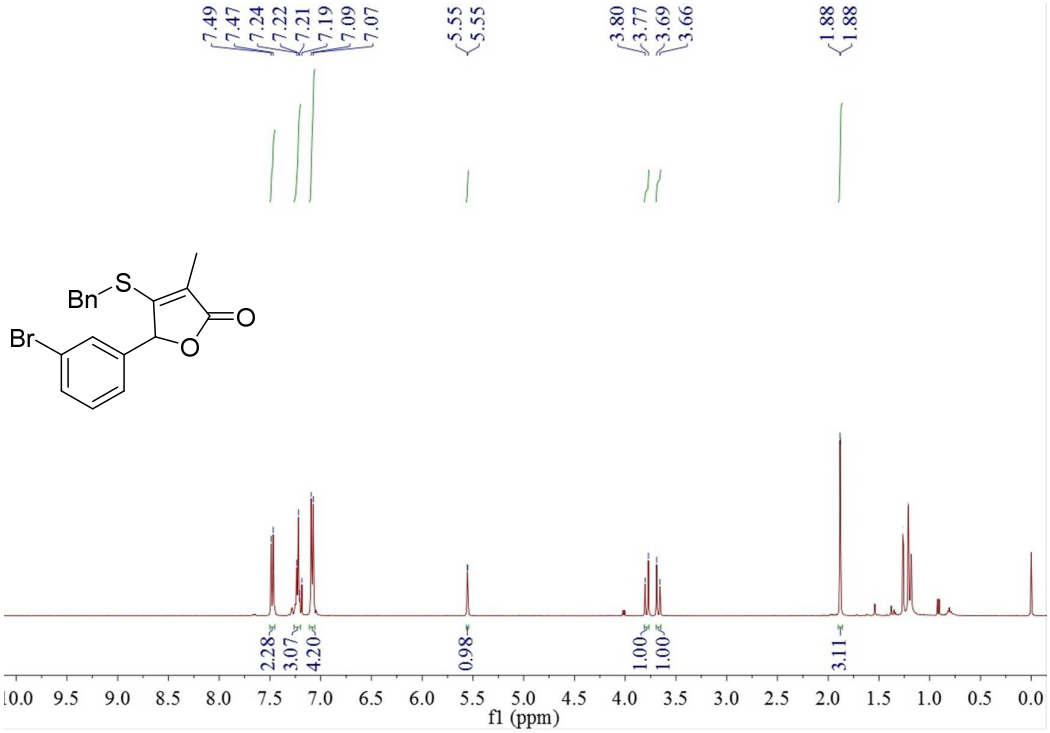


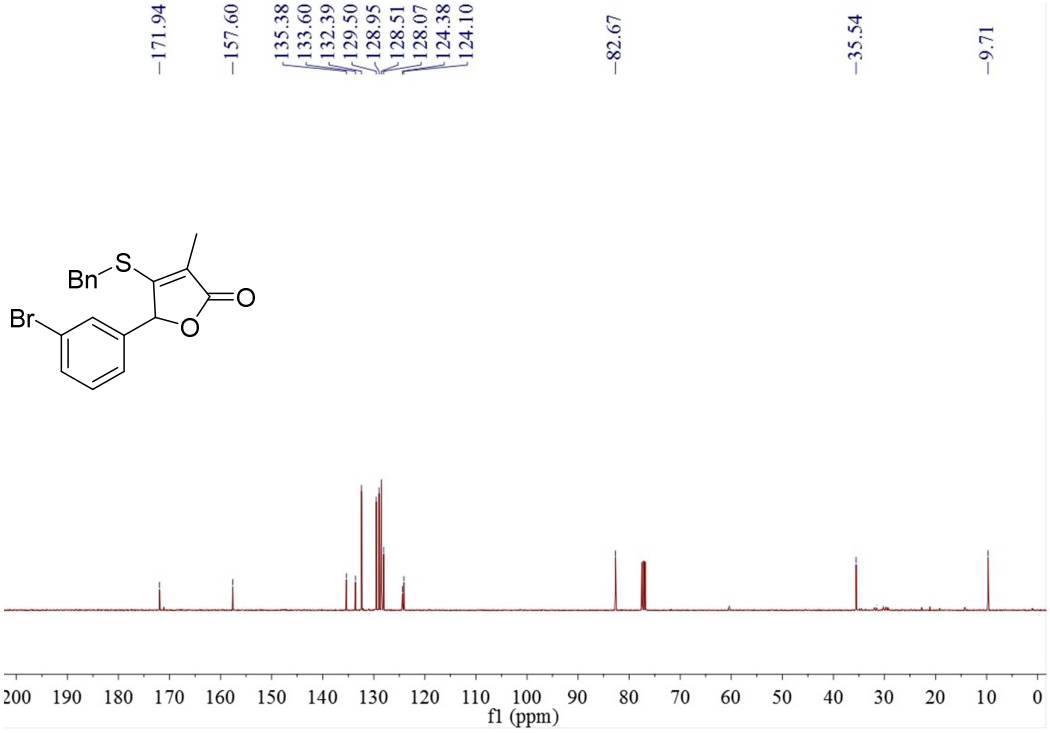
^{13}C NMR spectrum of **3e** in $CDCl_3$



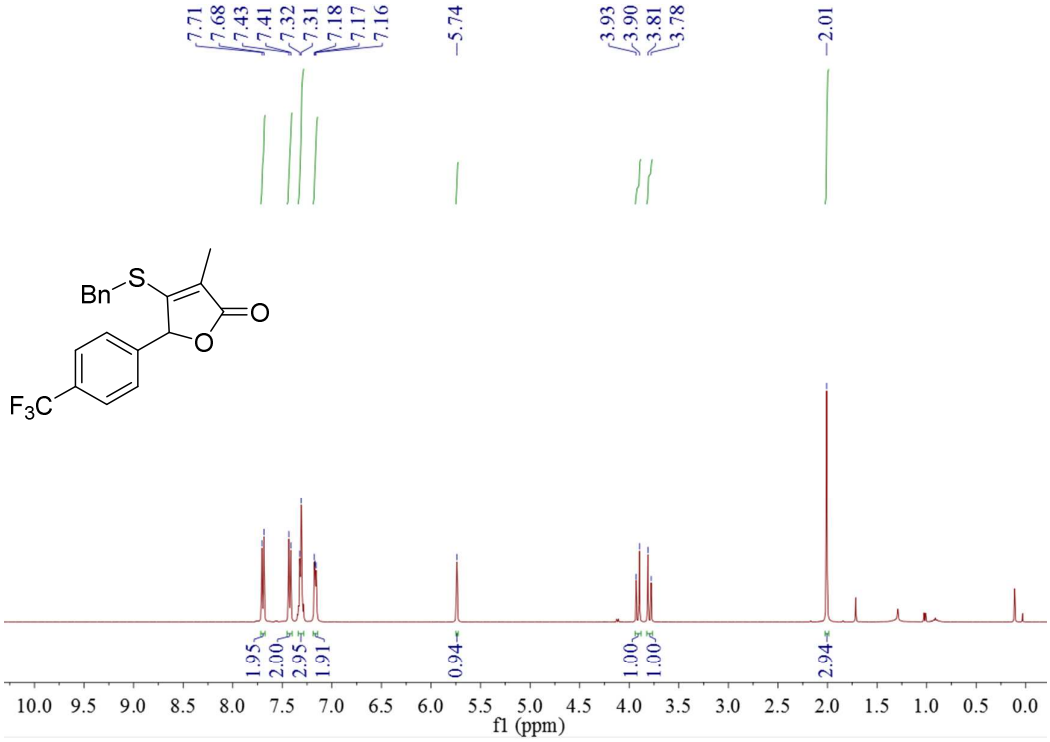
^{1}H NMR spectrum of **3f** in $CDCl_3$



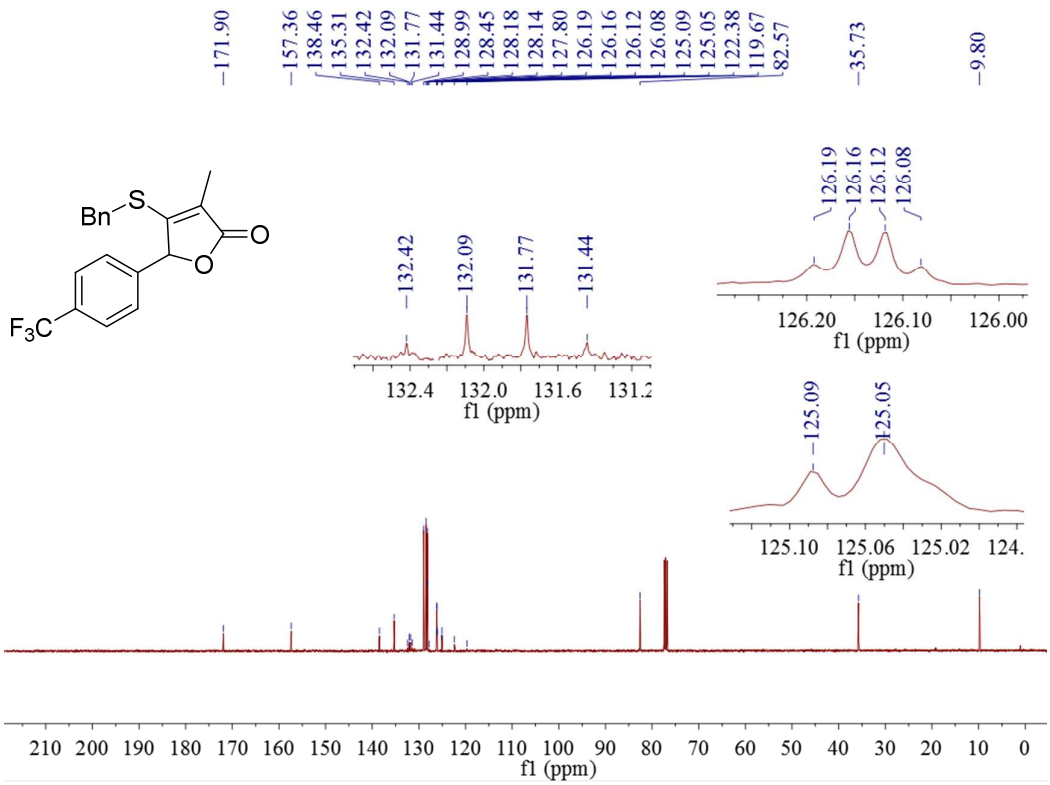
^{13}C NMR spectrum of **3f** in $CDCl_3$



^{1}H NMR spectrum of **3g** in $CDCl_3$



^{13}C NMR spectrum of **3g** in $CDCl_3$



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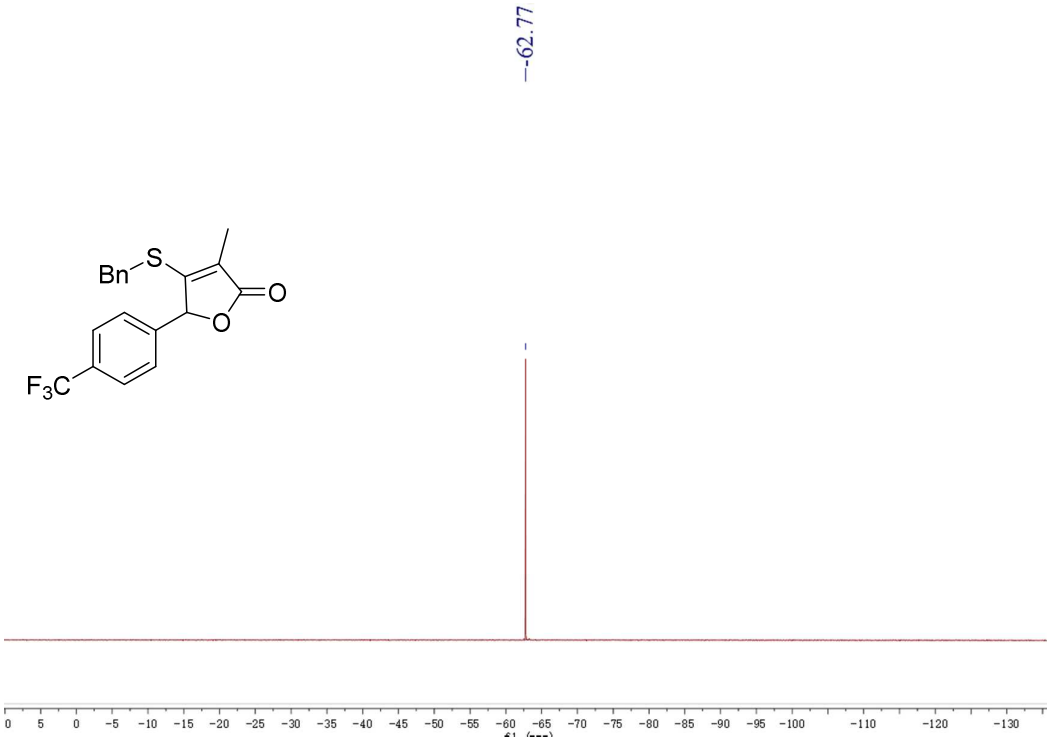

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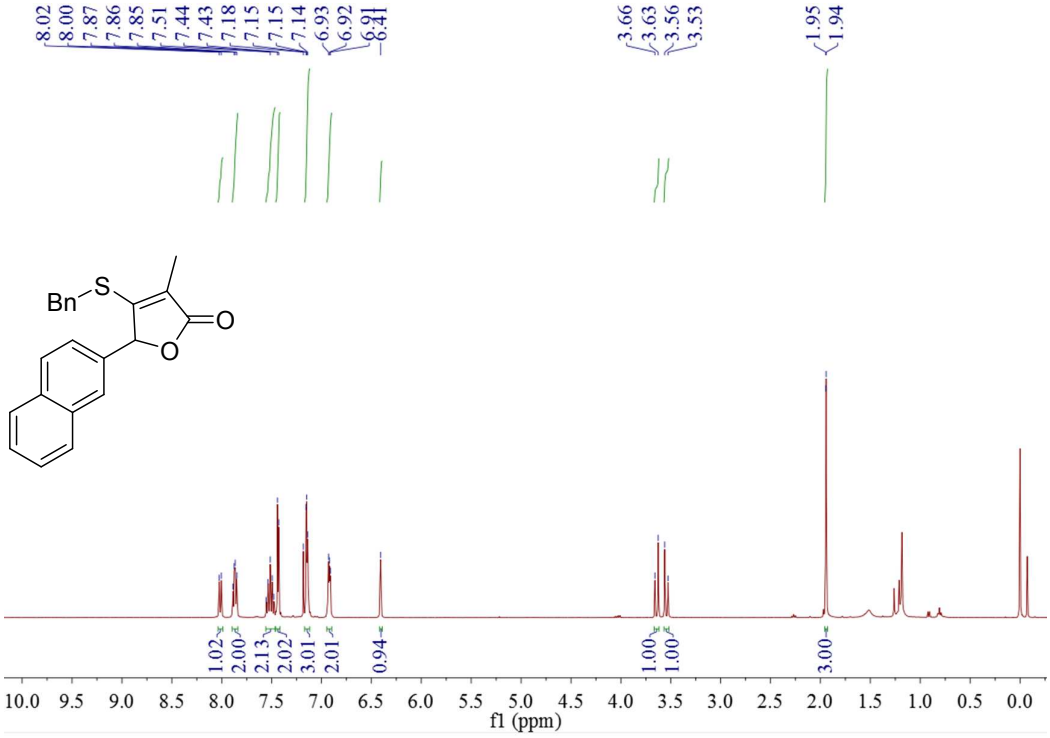
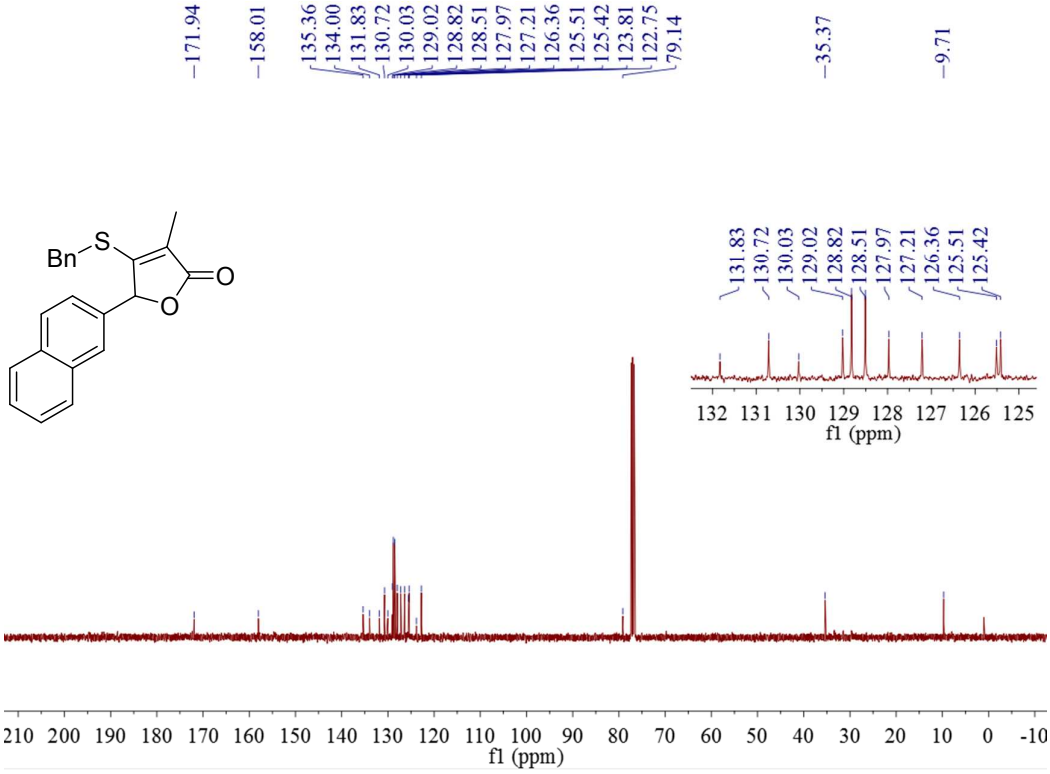
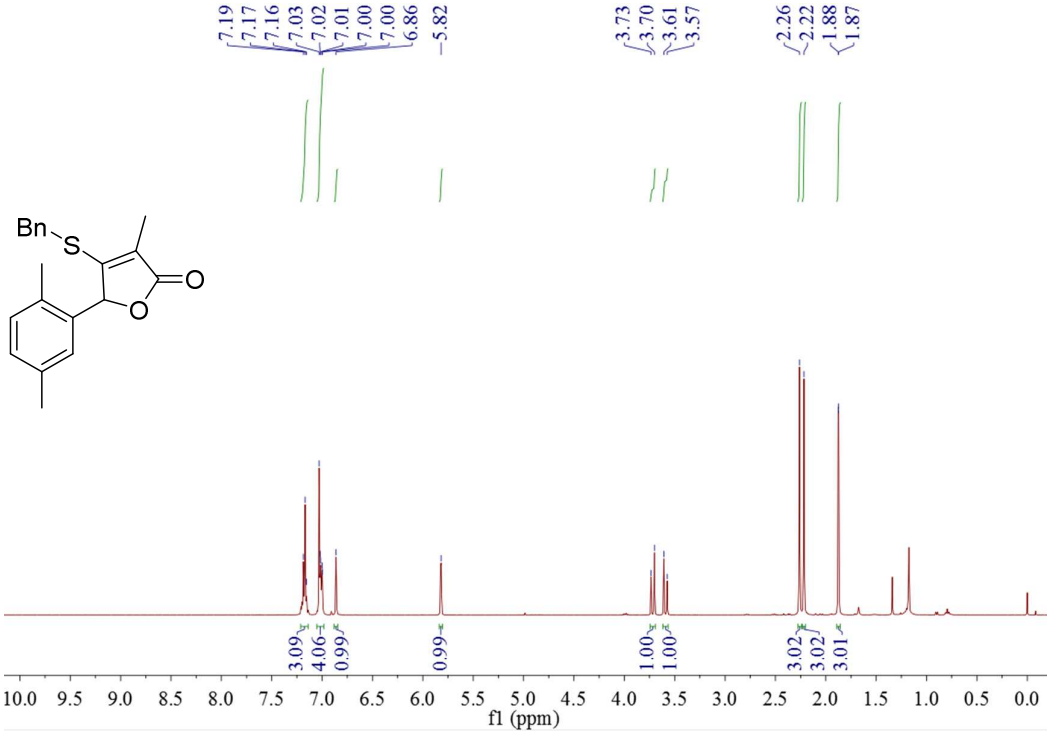


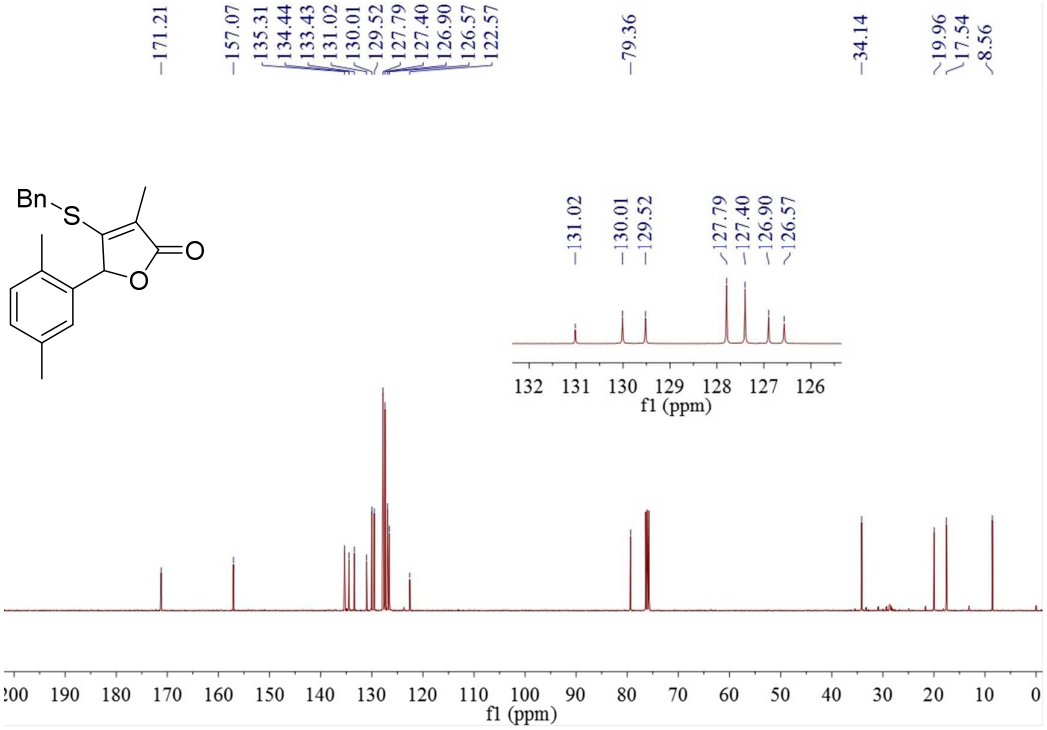
^{13}C NMR spectrum of **3h** in $CDCl_3$



^{1}H NMR spectrum of **3i** in $CDCl_3$



^{13}C NMR spectrum of **3i** in $CDCl_3$



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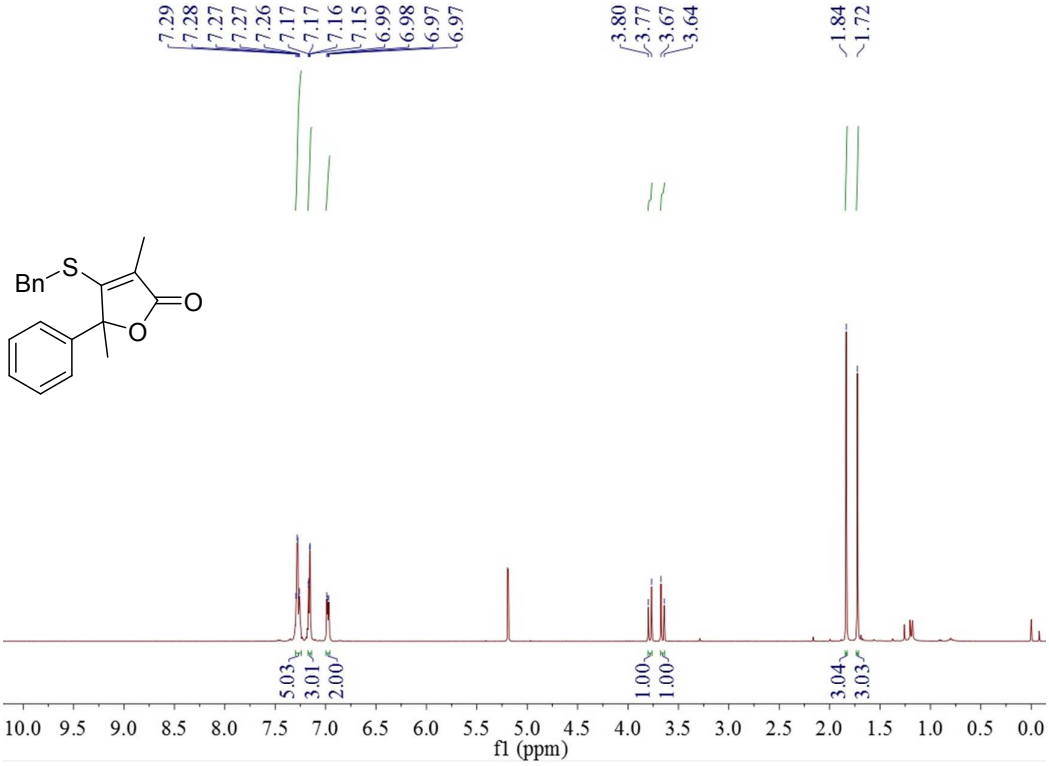

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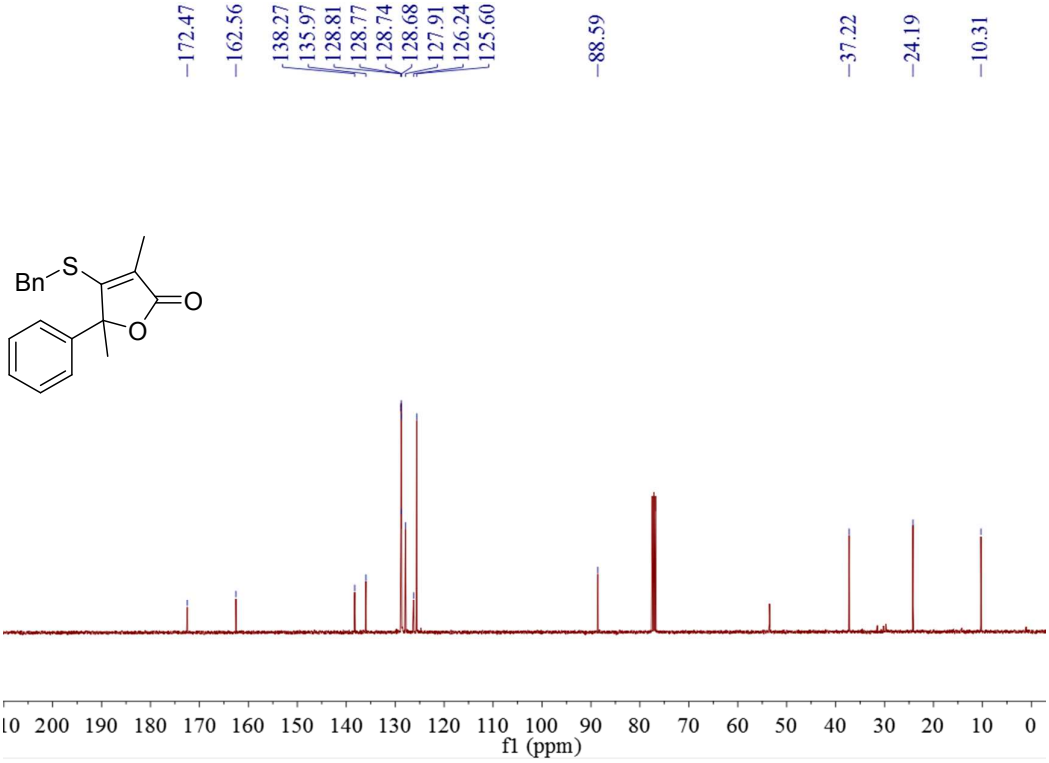

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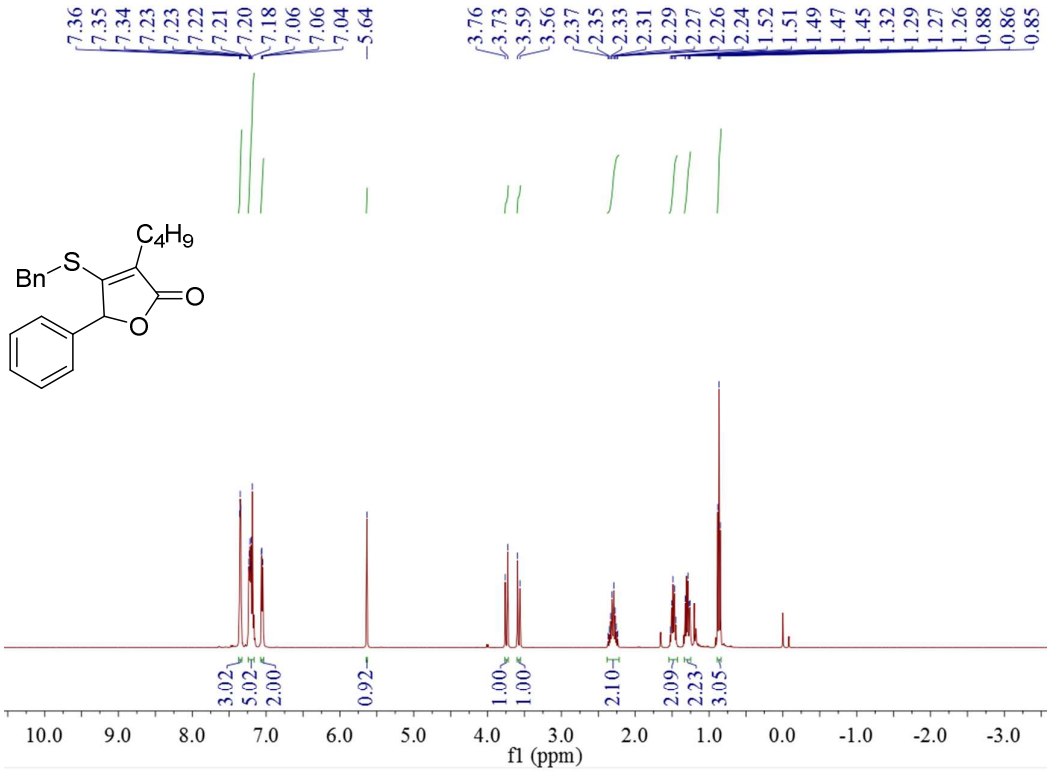

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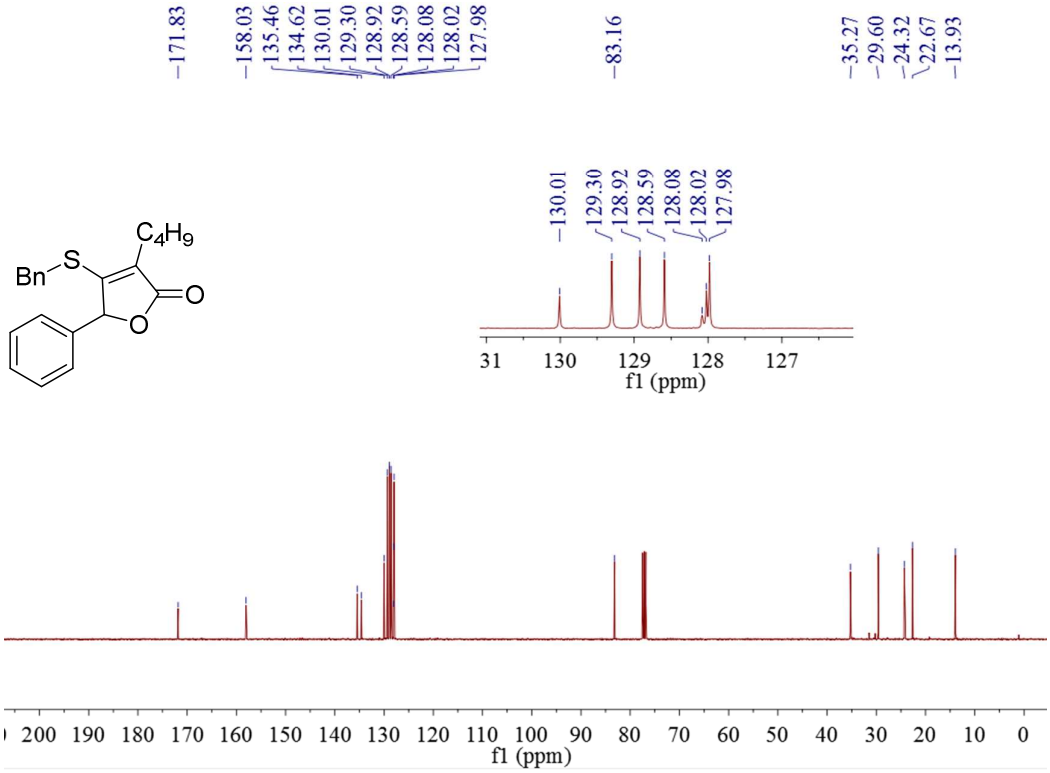

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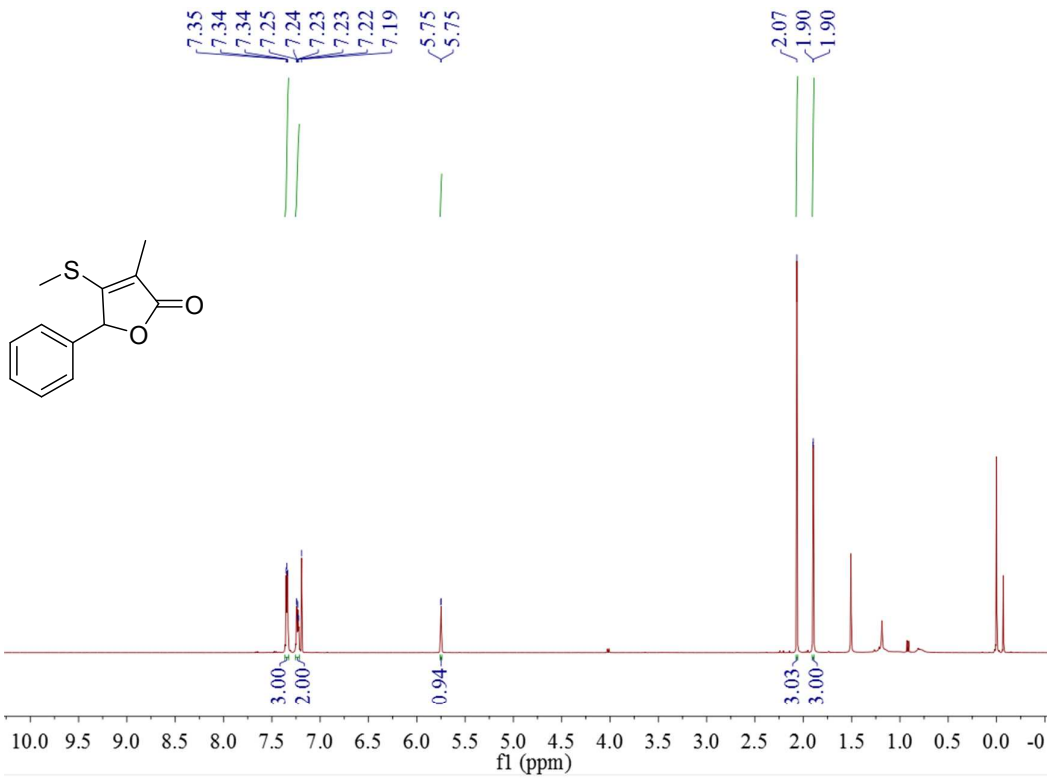
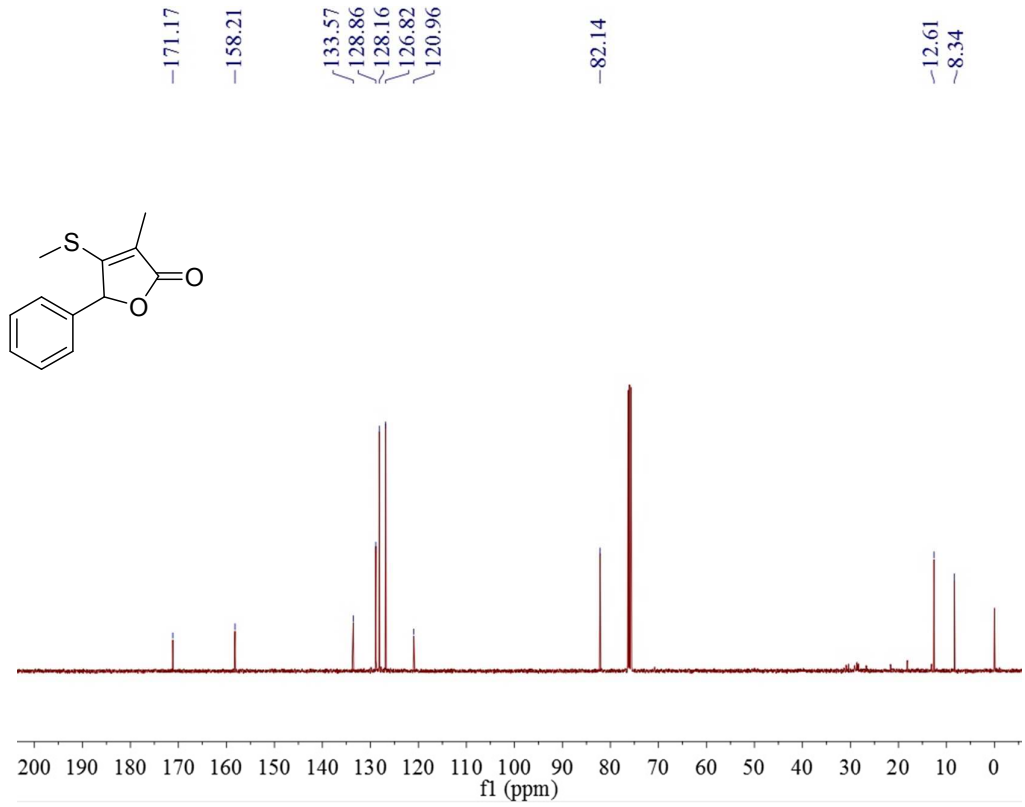
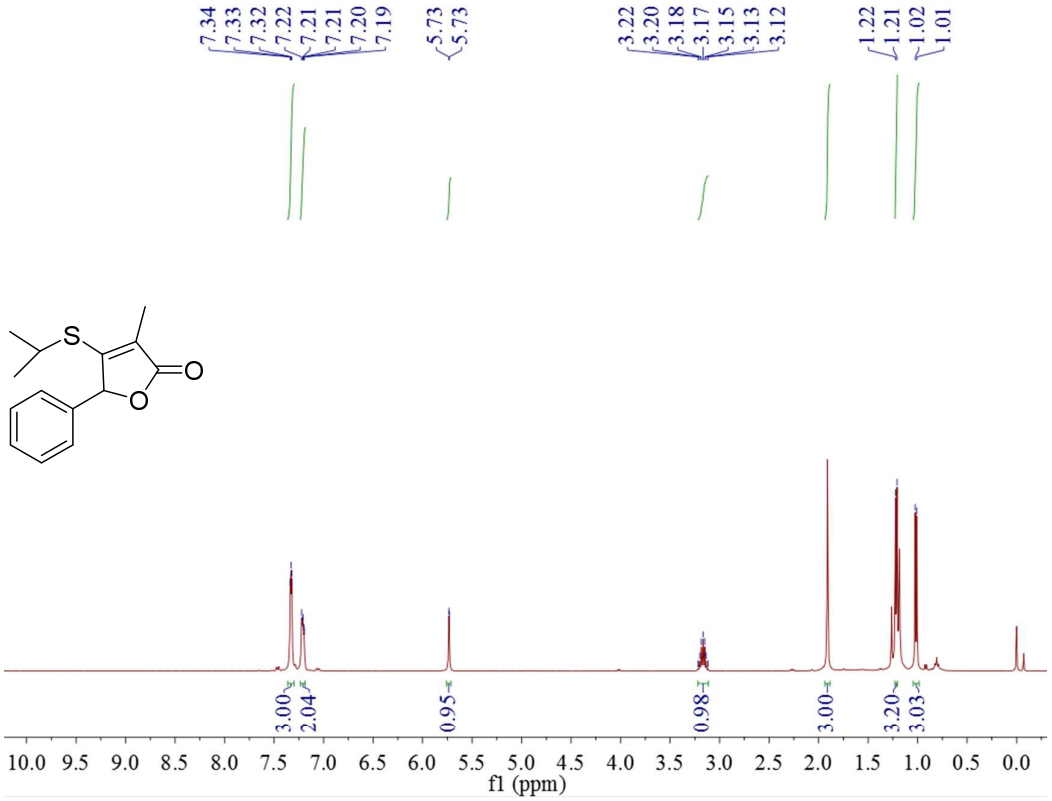


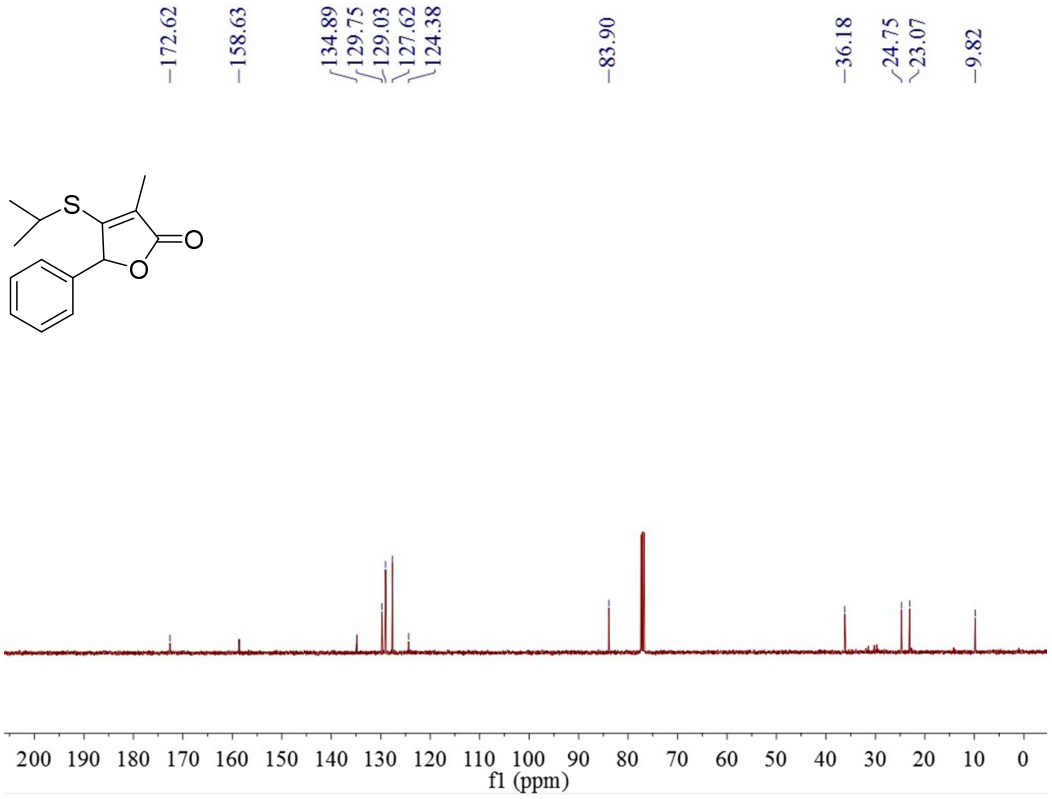
^{13}C NMR spectrum of **3l** in $CDCl_3$



^{1}H NMR spectrum of **3m** in $CDCl_3$



^{13}C NMR spectrum of **3m** in $CDCl_3$



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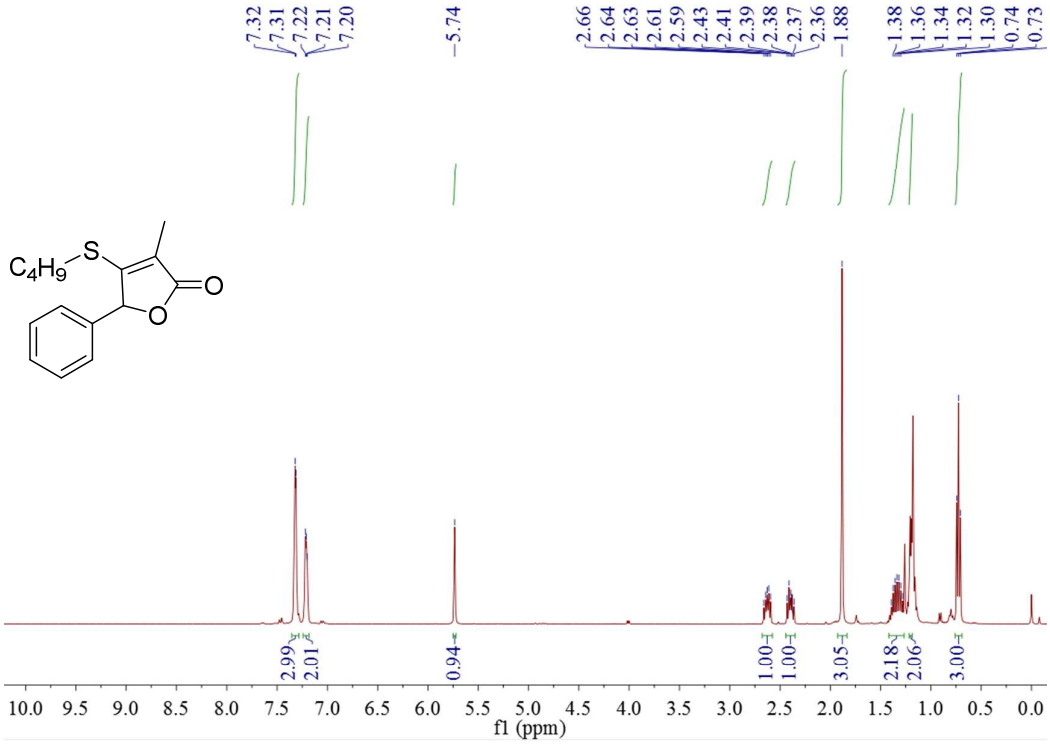

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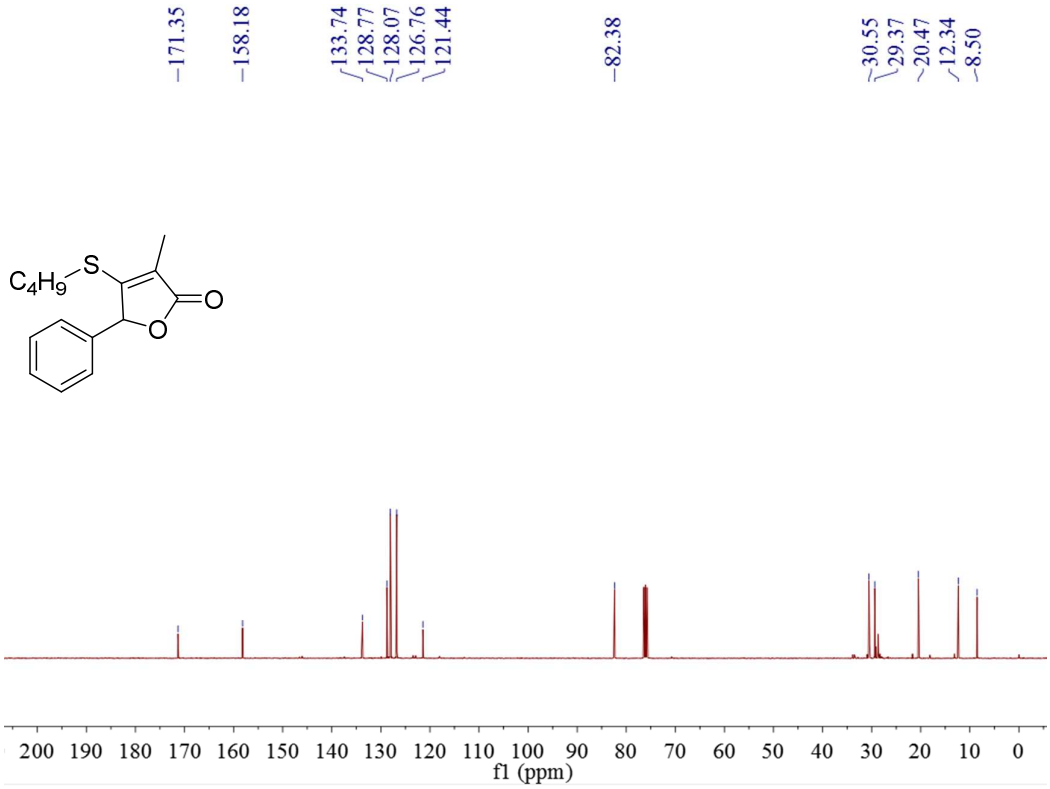

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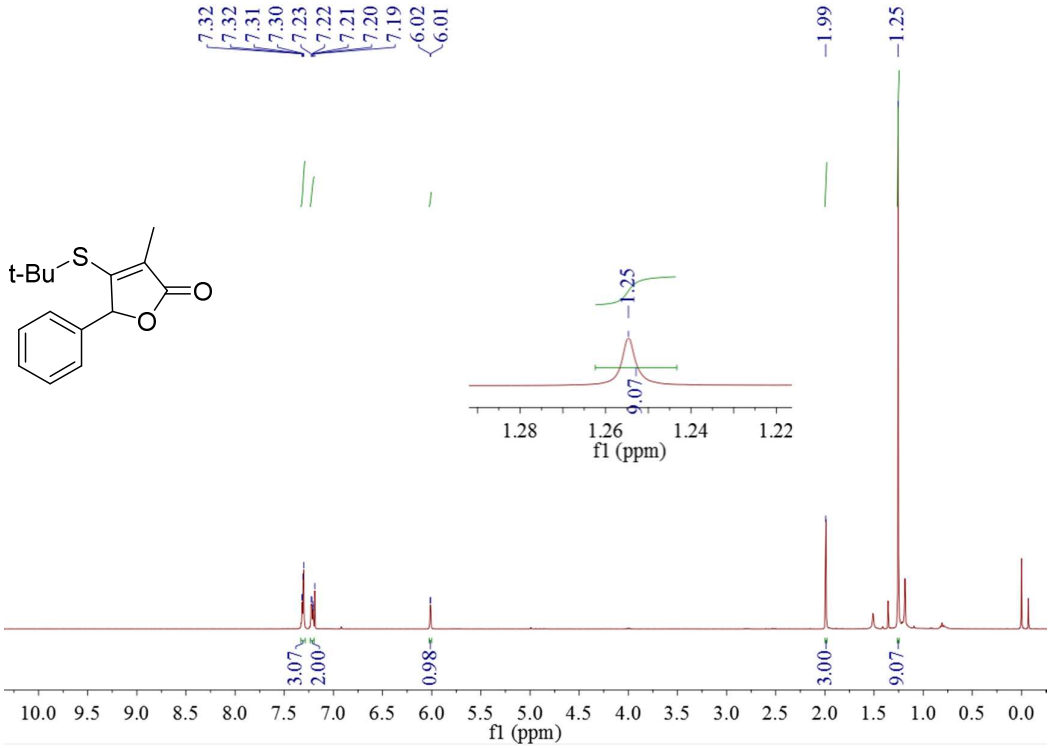

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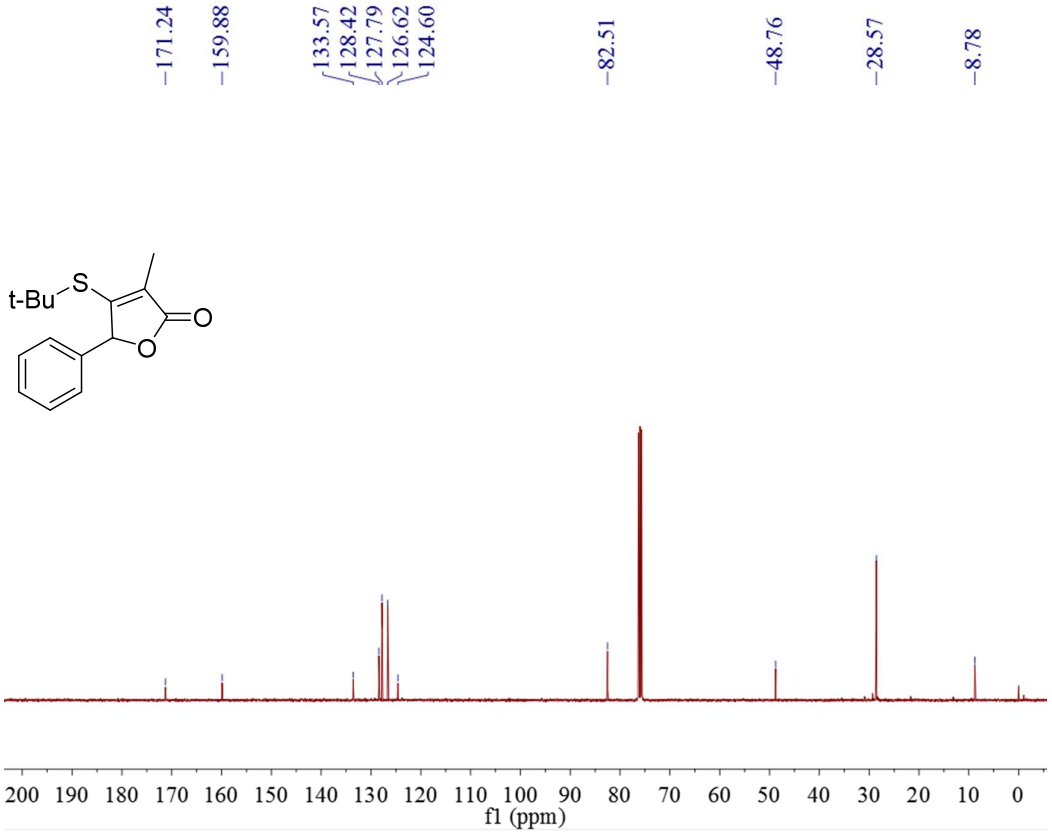

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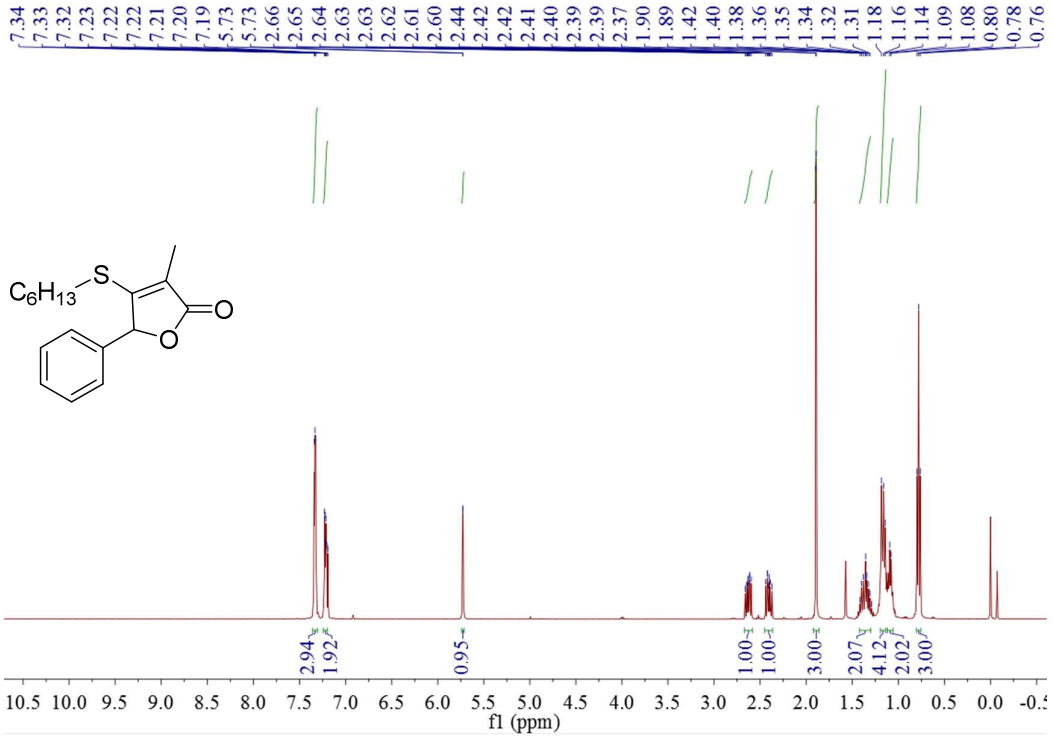

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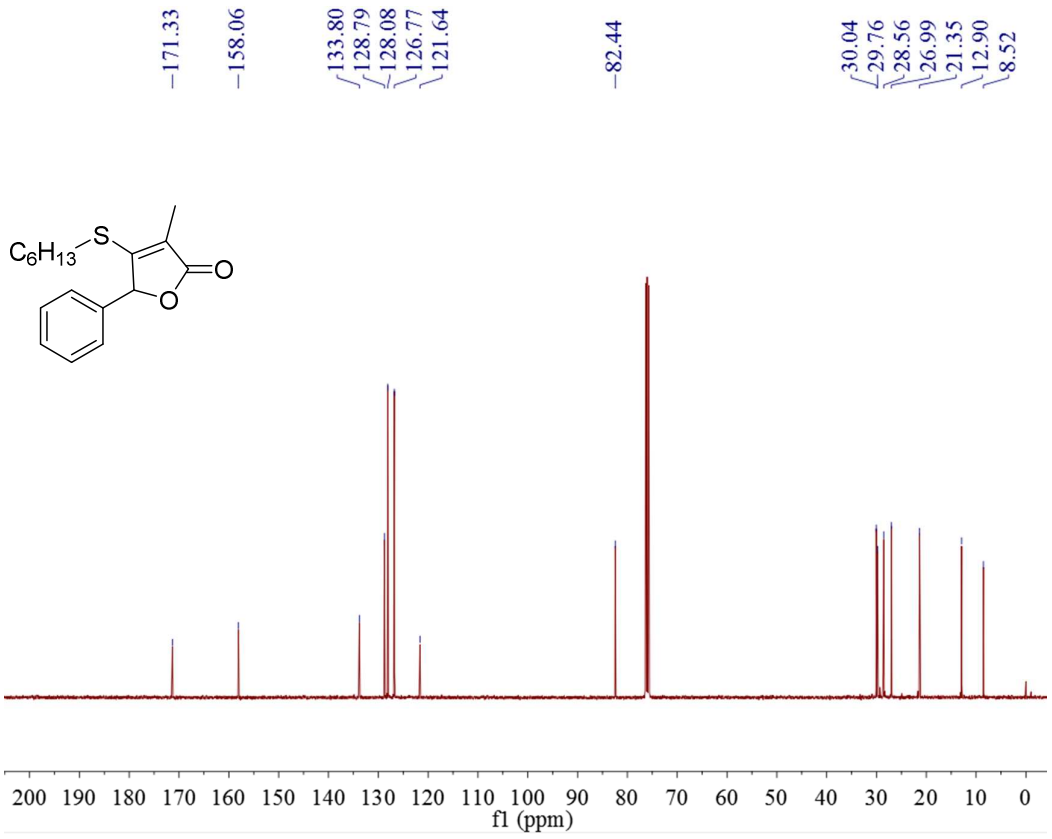

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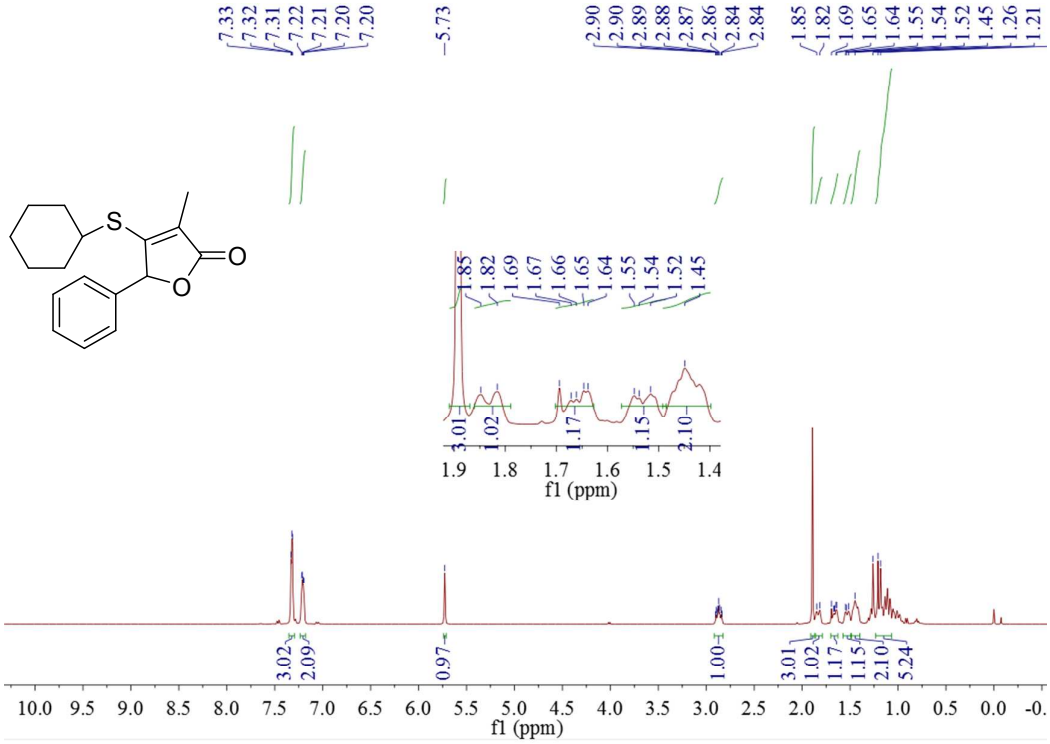

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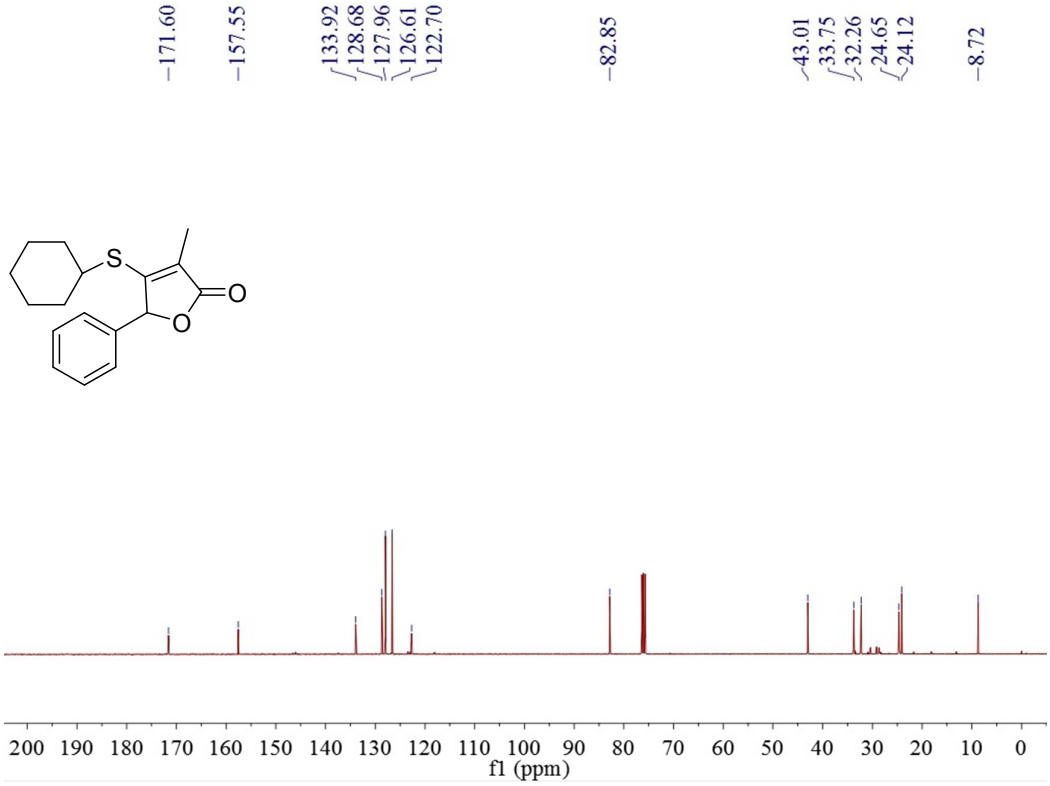

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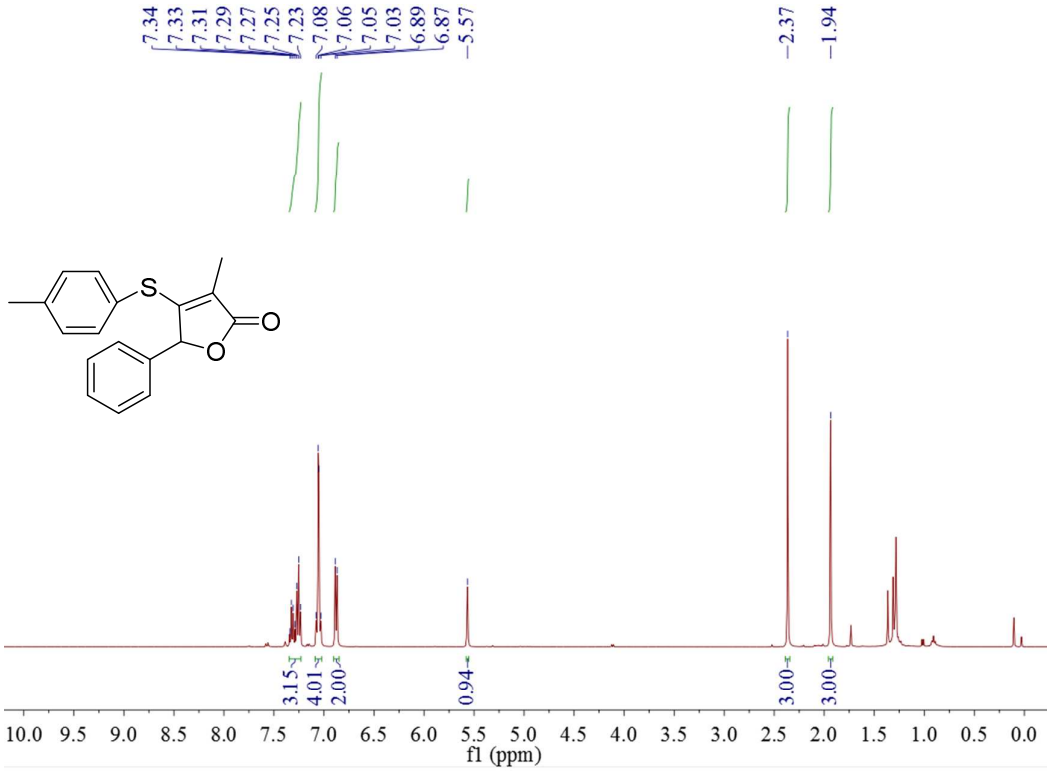

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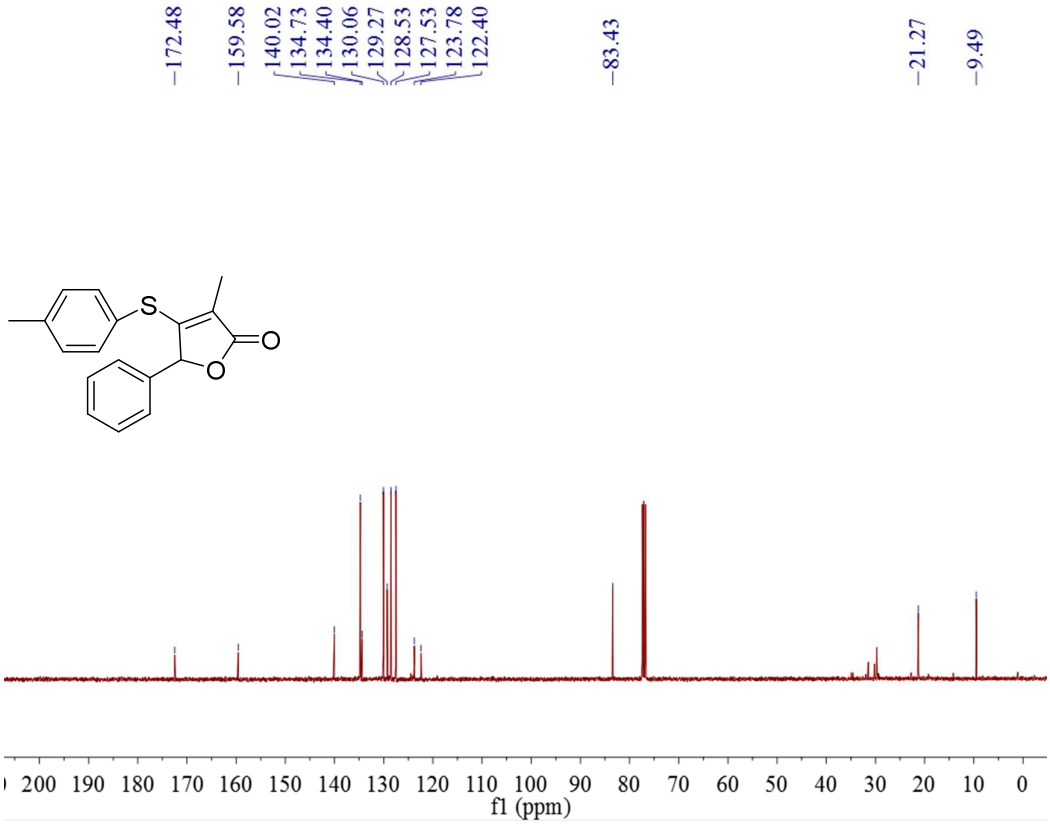

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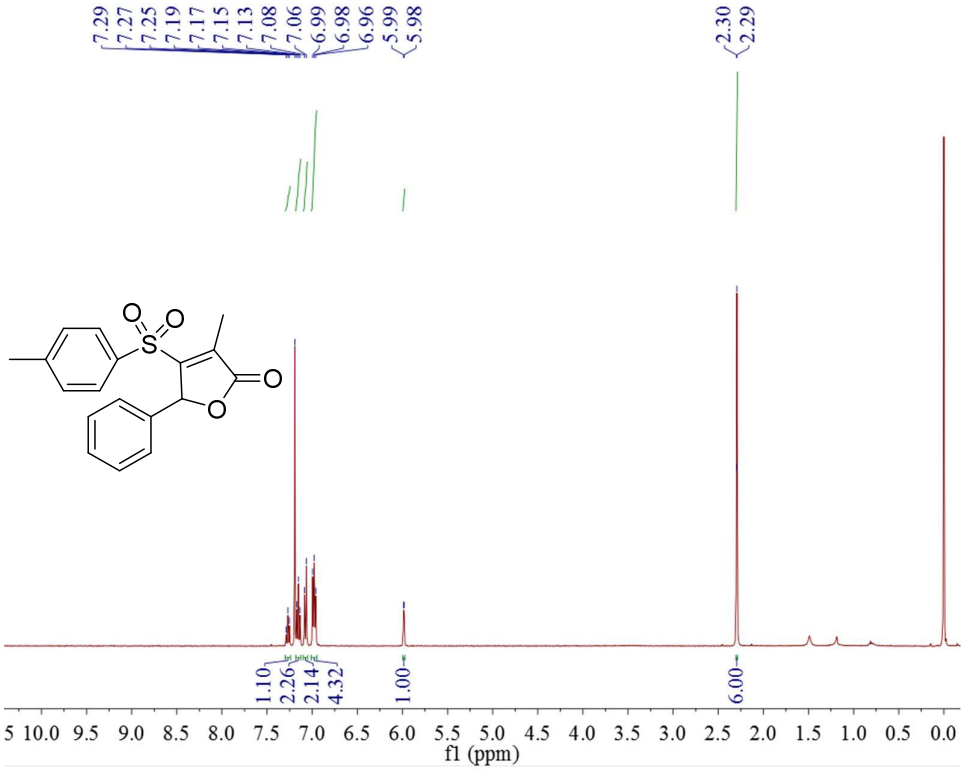

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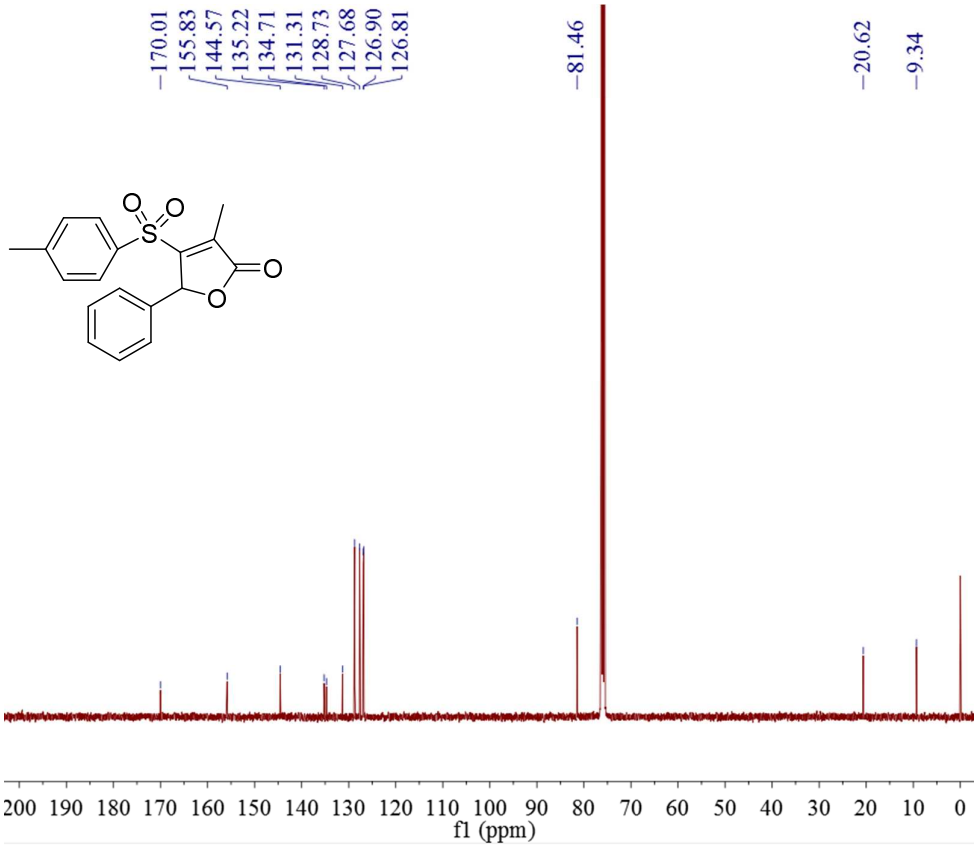

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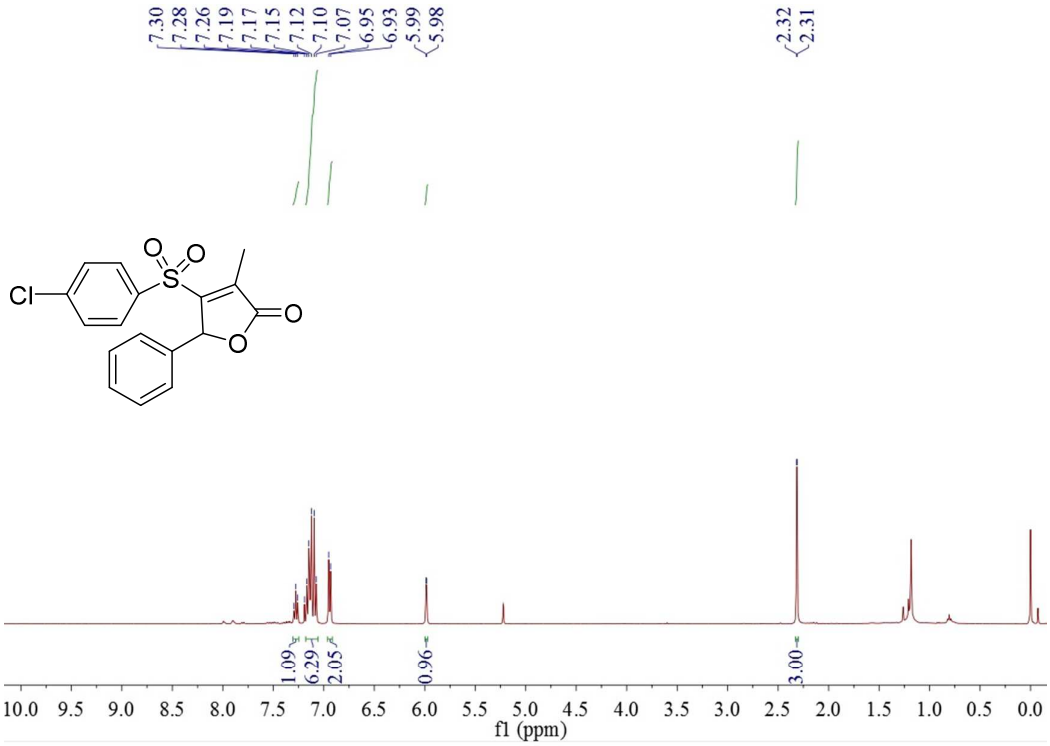
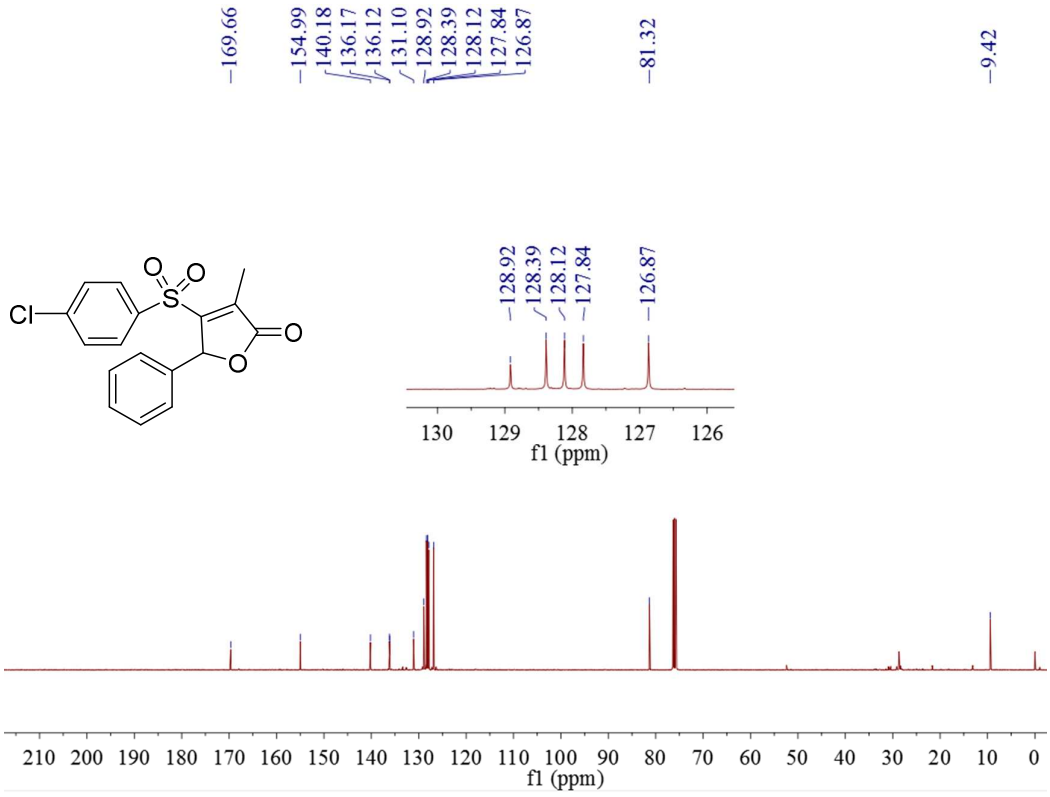
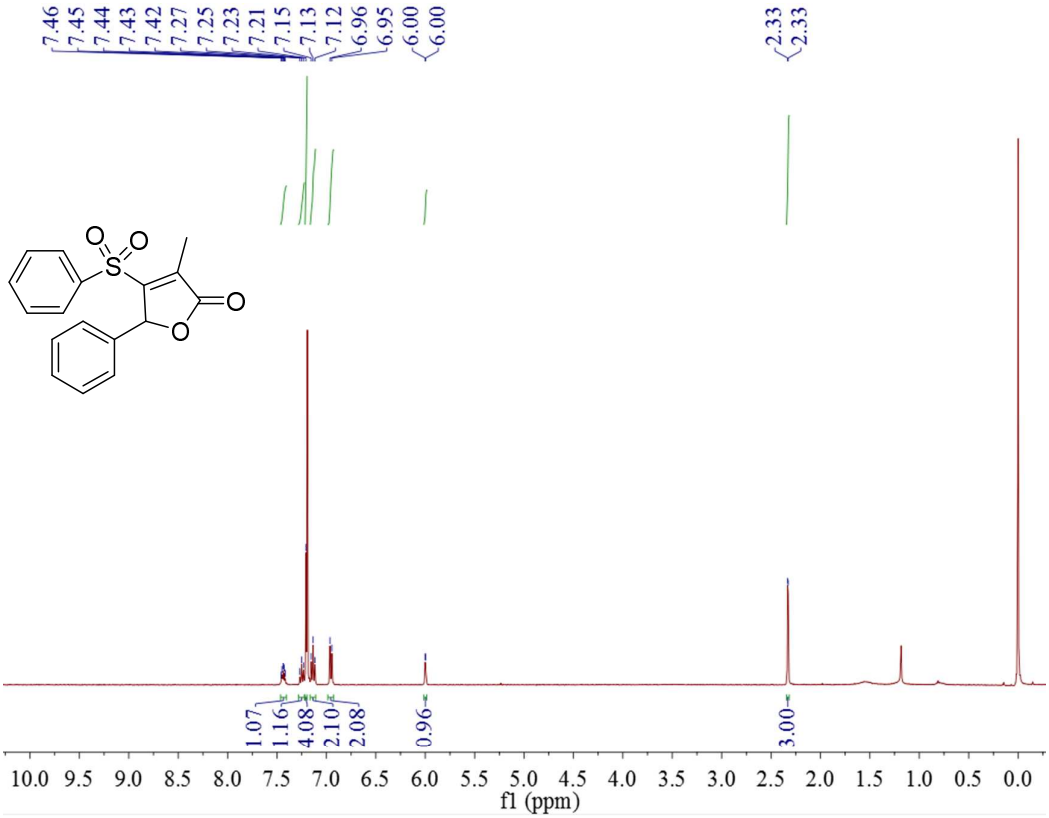


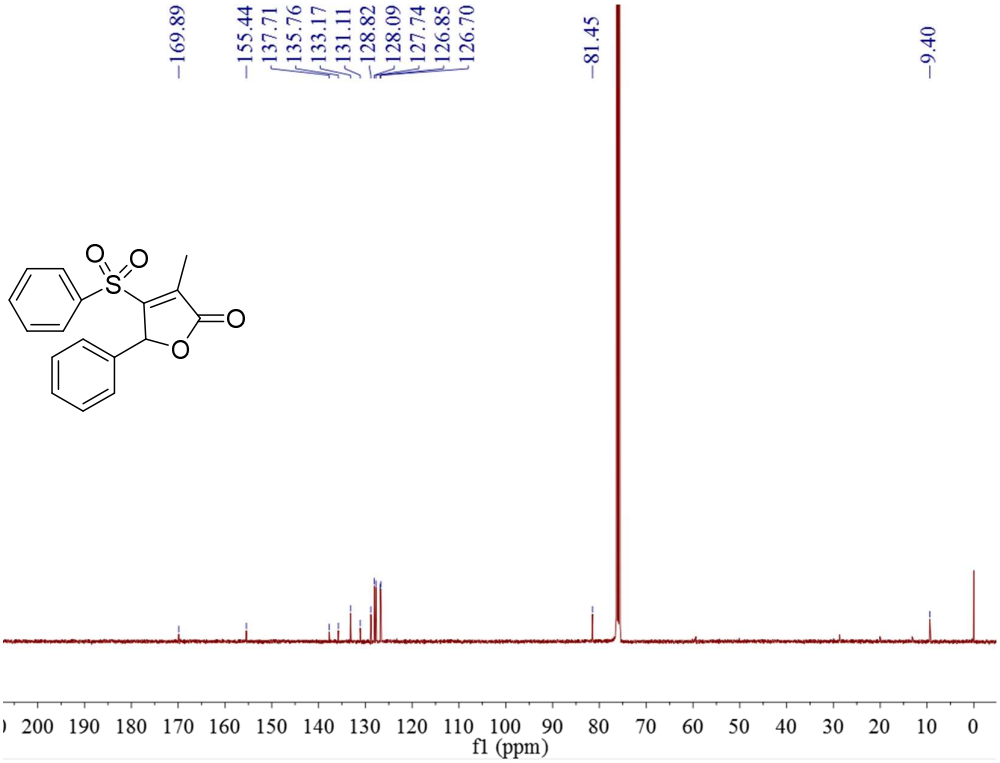
^{13}C NMR spectrum of **4b** in $CDCl_3$



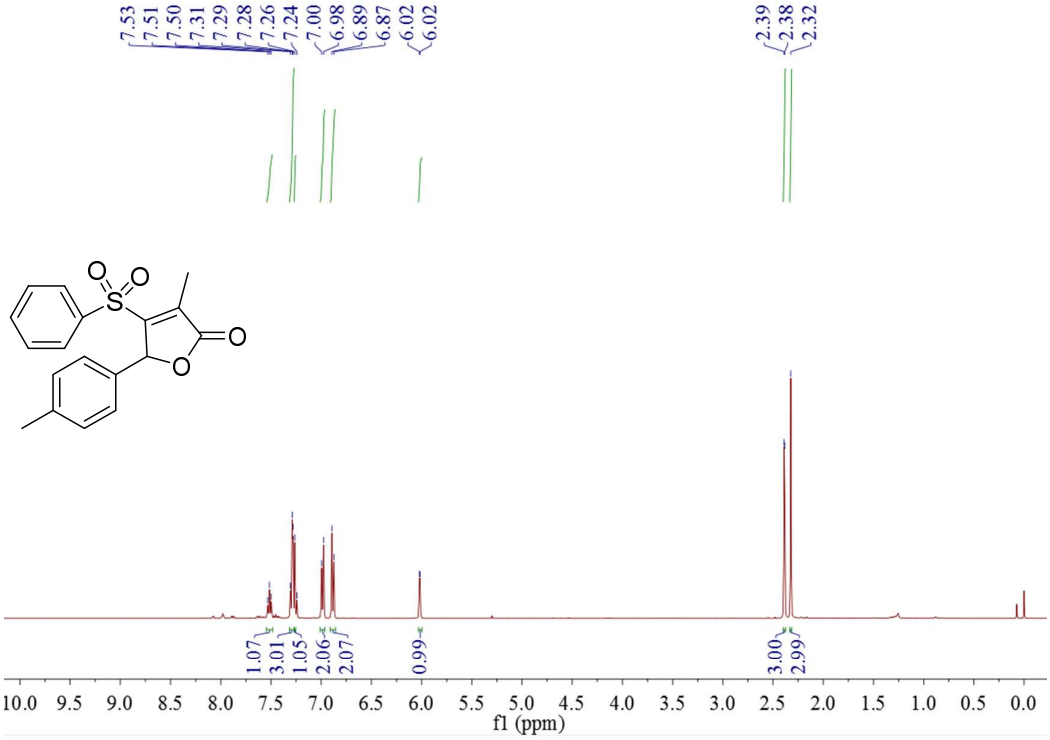
^{1}H NMR spectrum of **4c** in $CDCl_3$



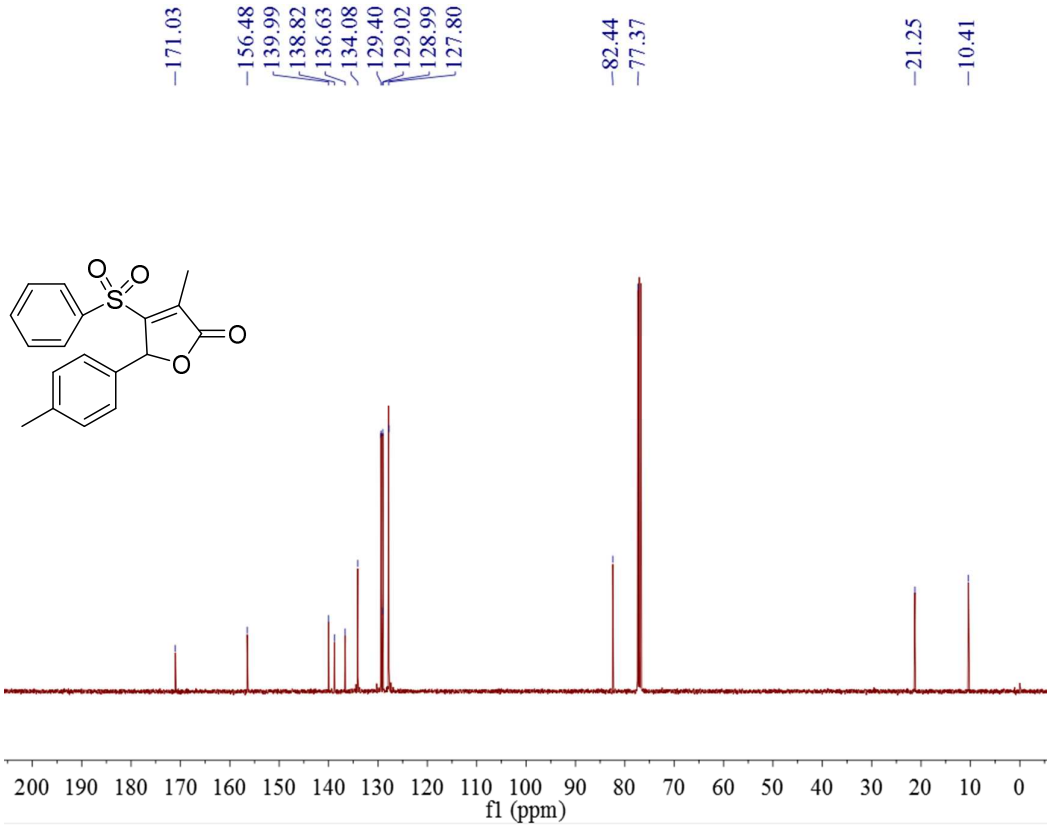
^{13}C NMR spectrum of **4c** in $CDCl_3$



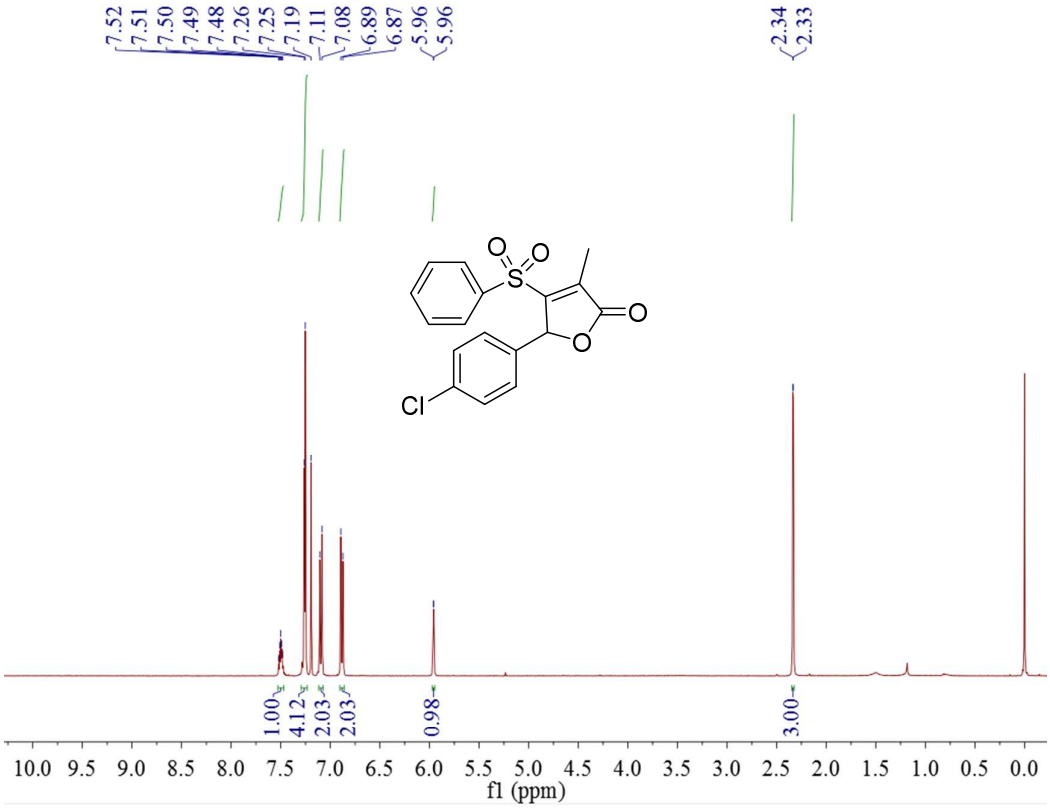
^{1}H NMR spectrum of **4d** in $CDCl_3$



^{13}C NMR spectrum of **4d** in $CDCl_3$



^{1}H NMR spectrum of **4e** in $CDCl_3$



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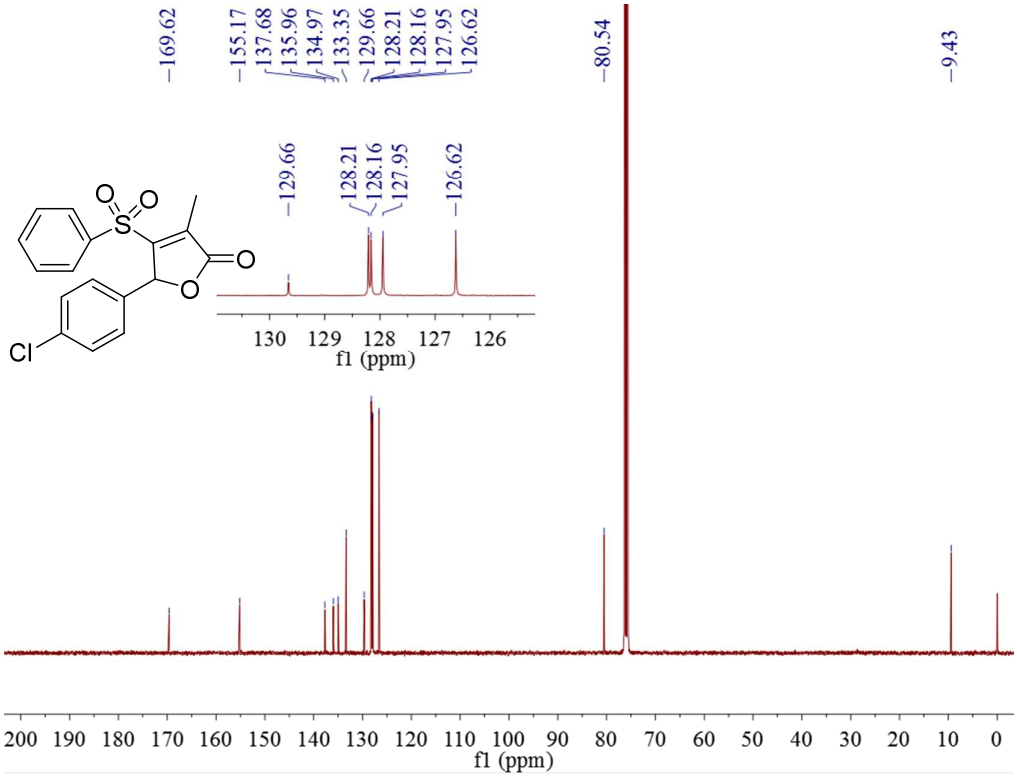
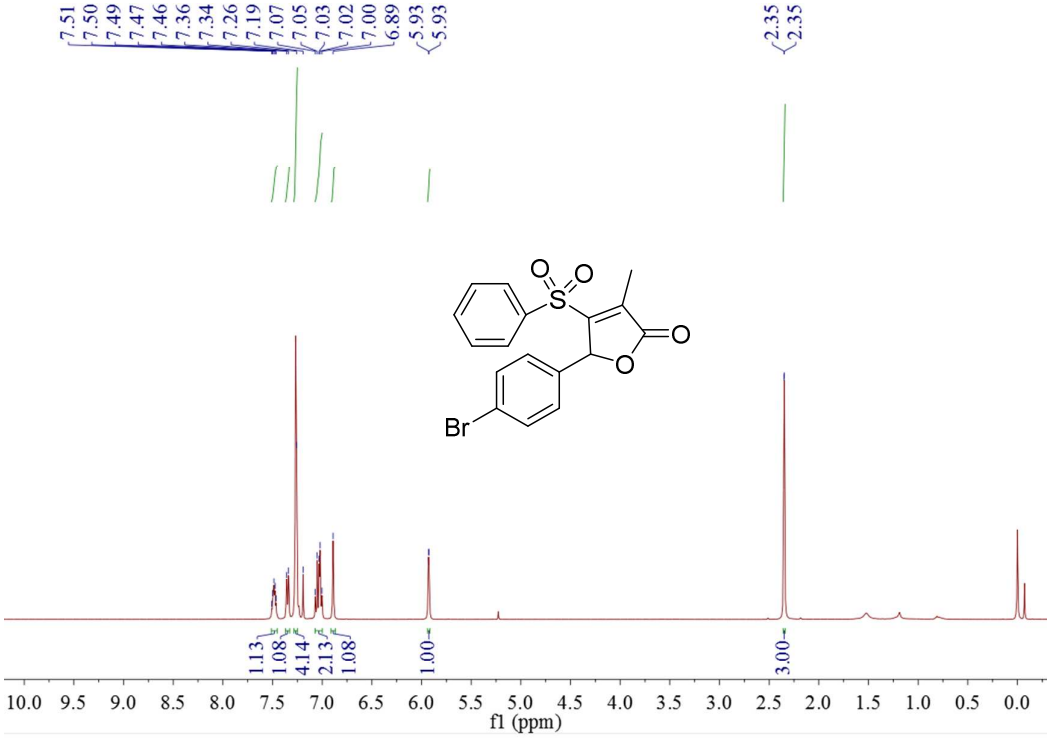
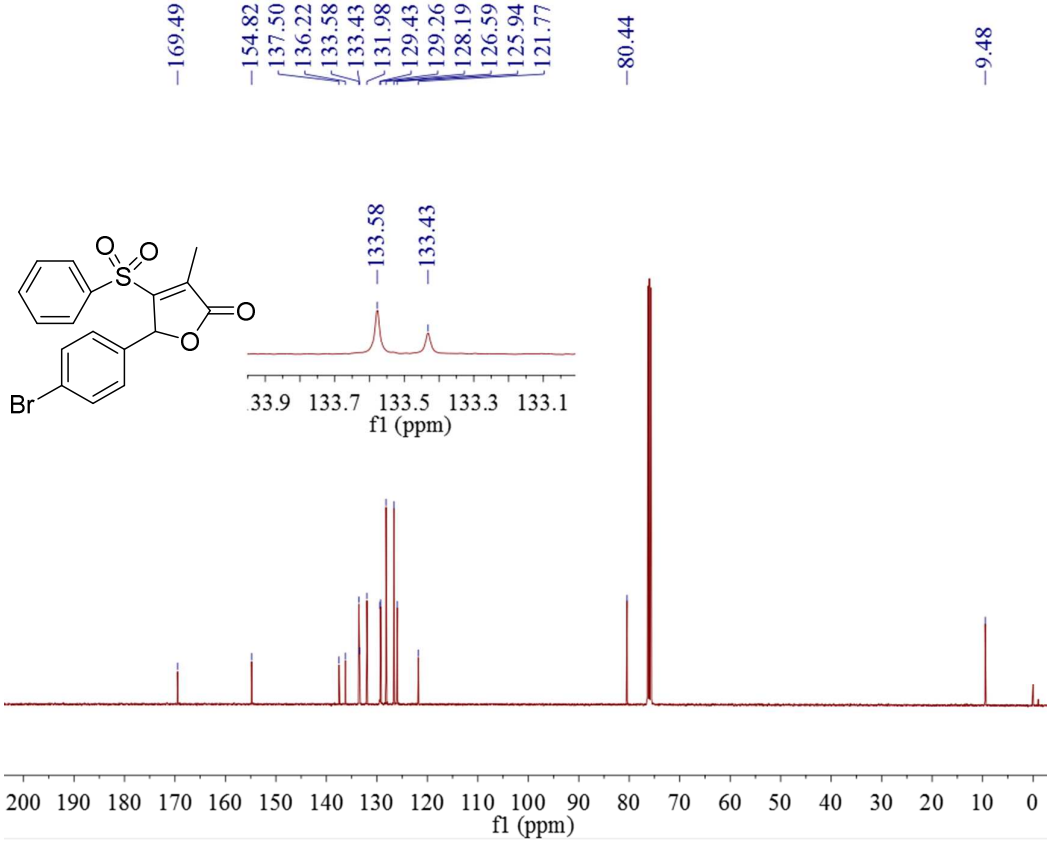


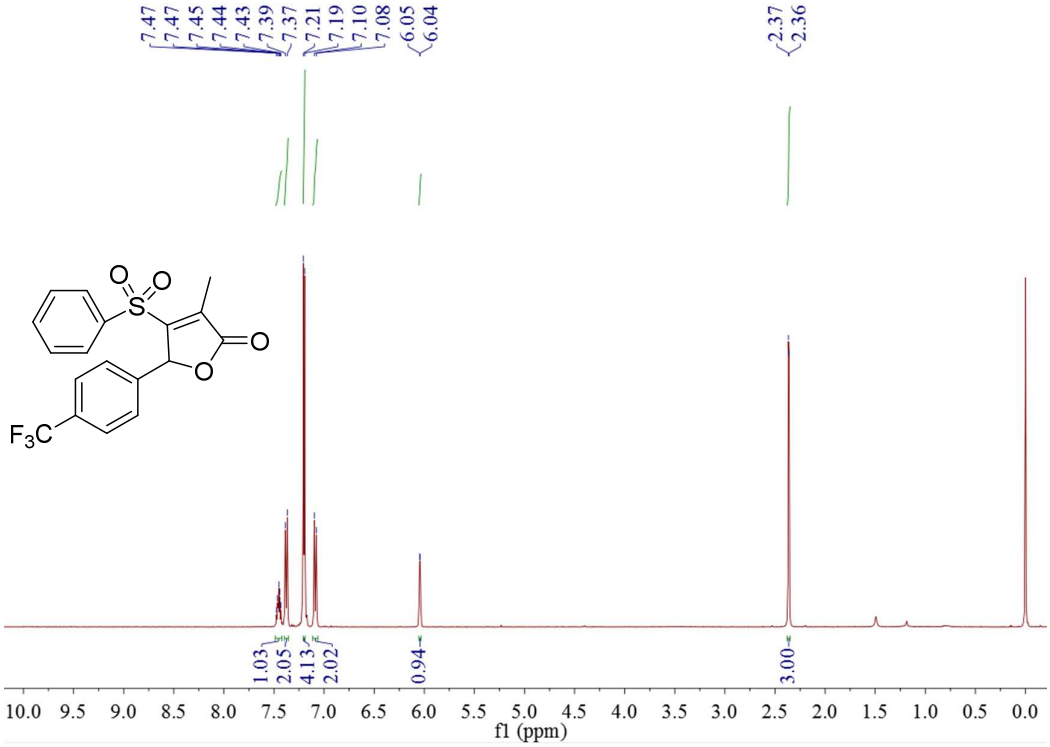
^{1}H NMR spectrum of **4f** in $CDCl_3$



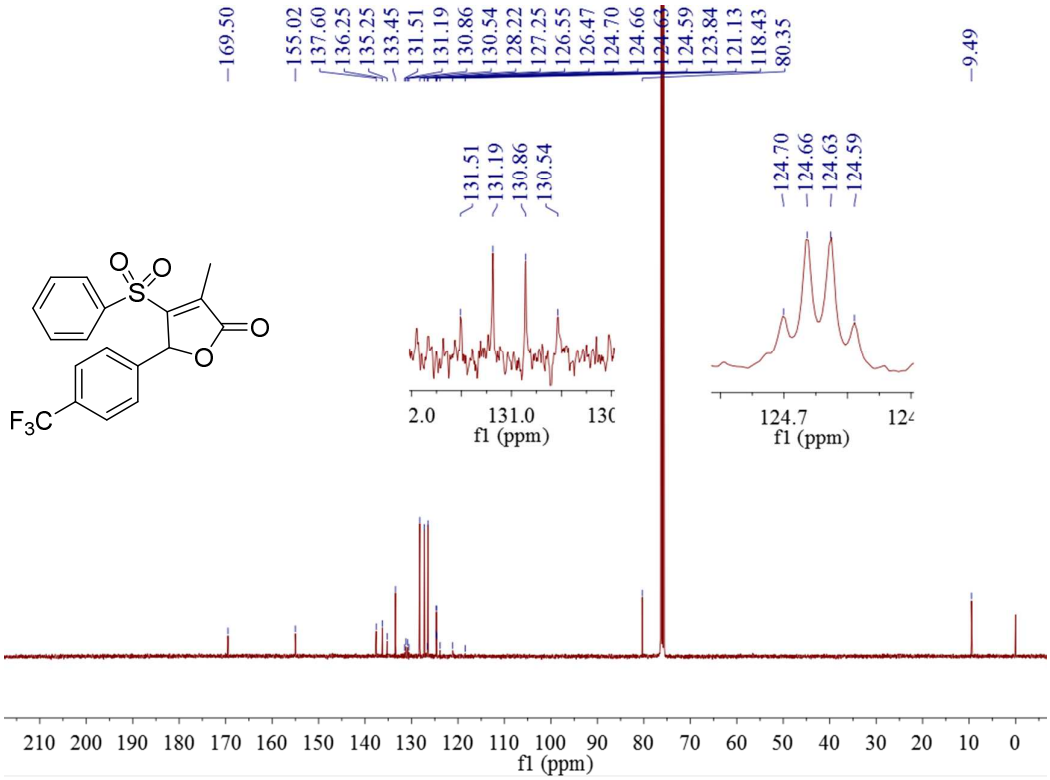
^{13}C NMR spectrum of **4f** in $CDCl_3$



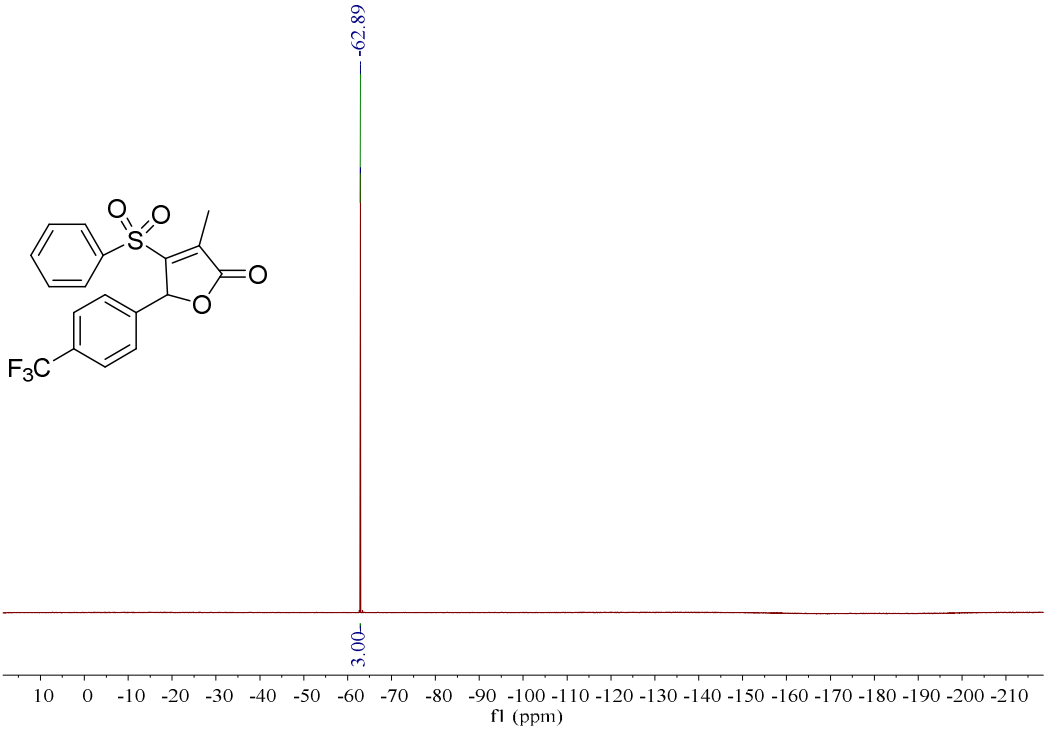
^{1}H NMR spectrum of **4g** in $CDCl_3$



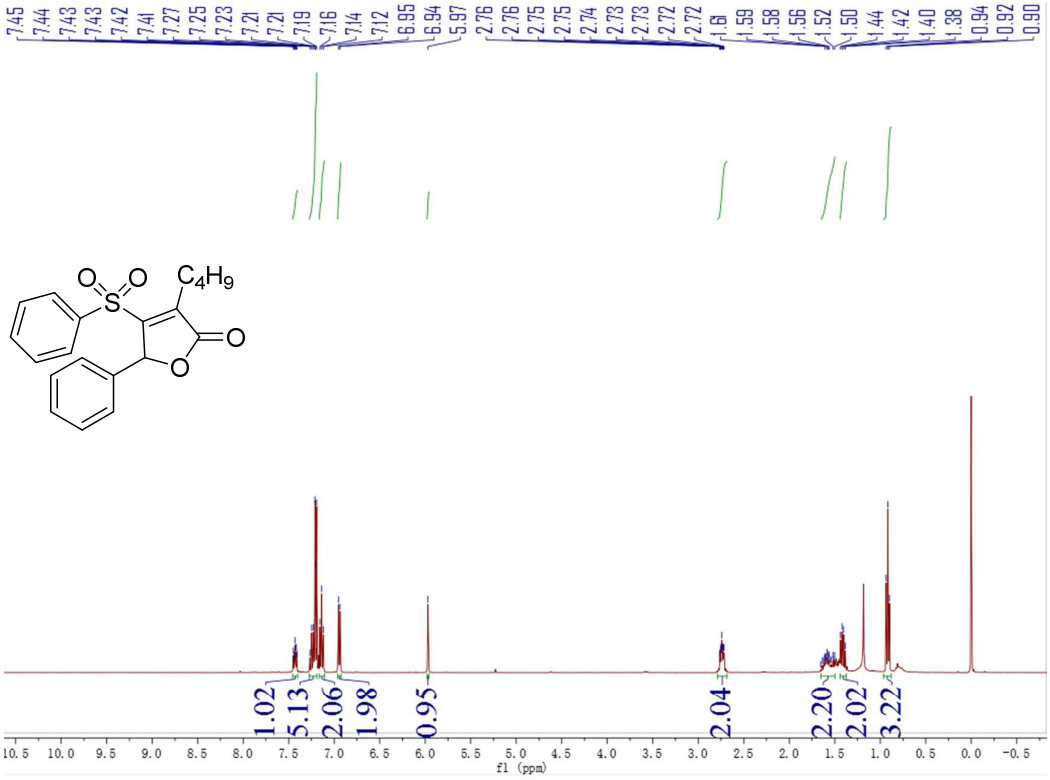
^{13}C NMR spectrum of **4g** in $CDCl_3$



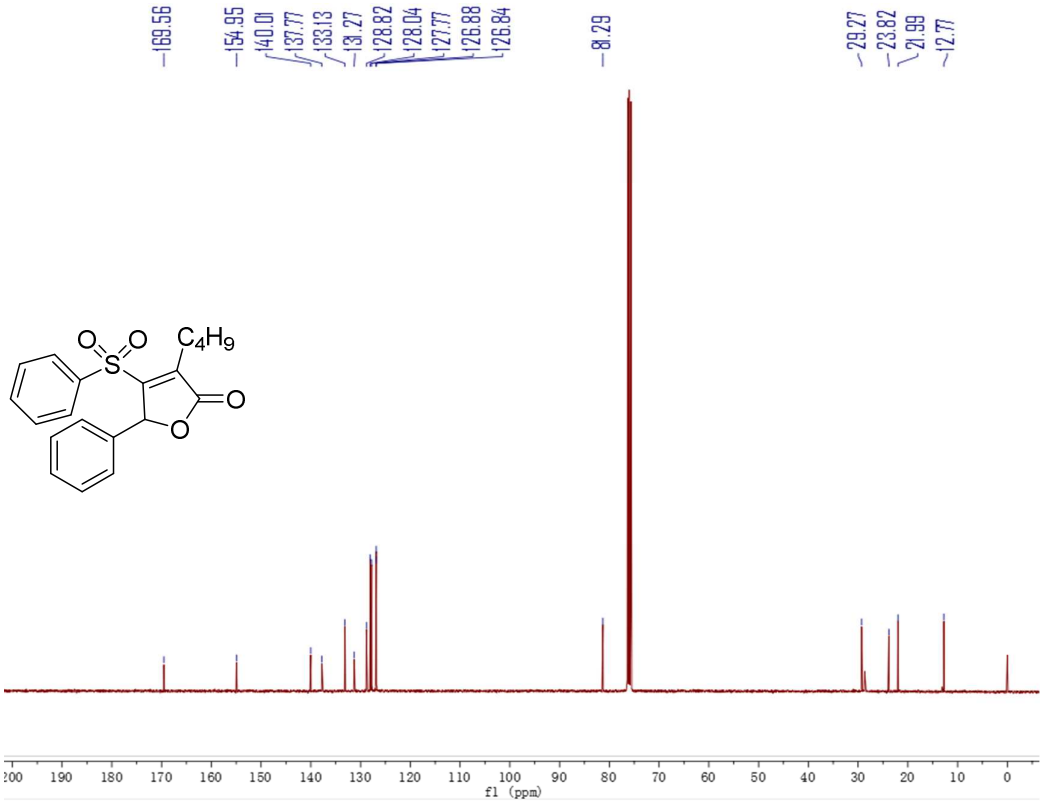
^{19}F NMR spectrum of **4g** in $CDCl_3$



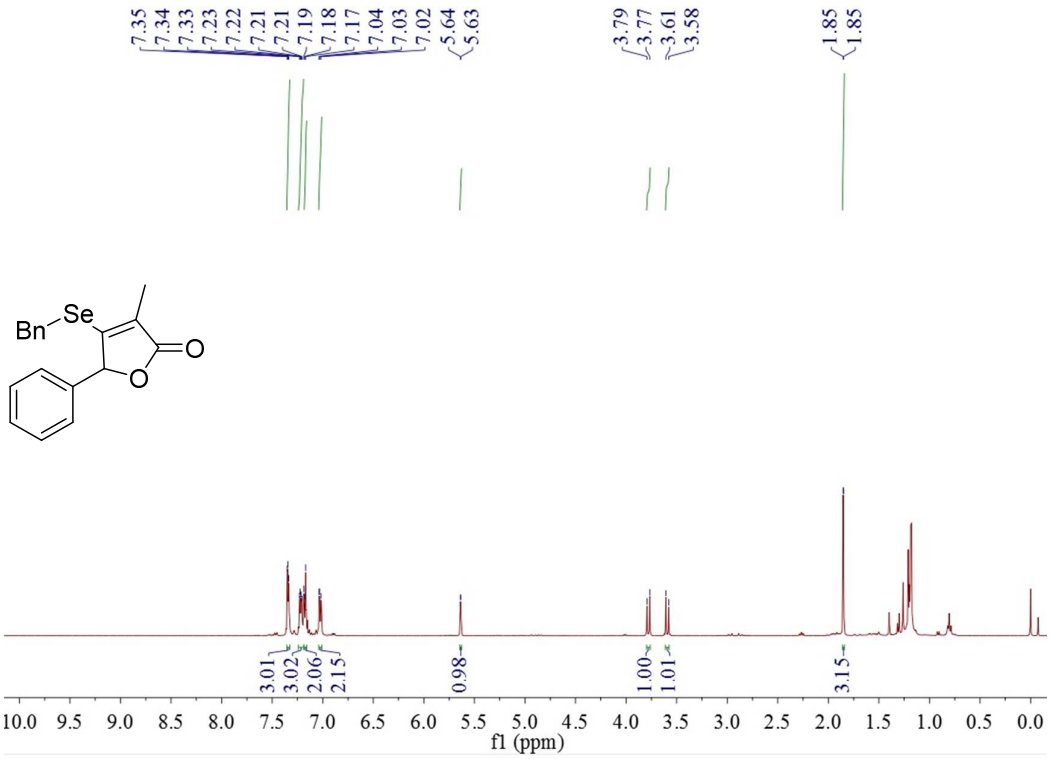
^{1}H NMR spectrum of **4h** in $CDCl_3$



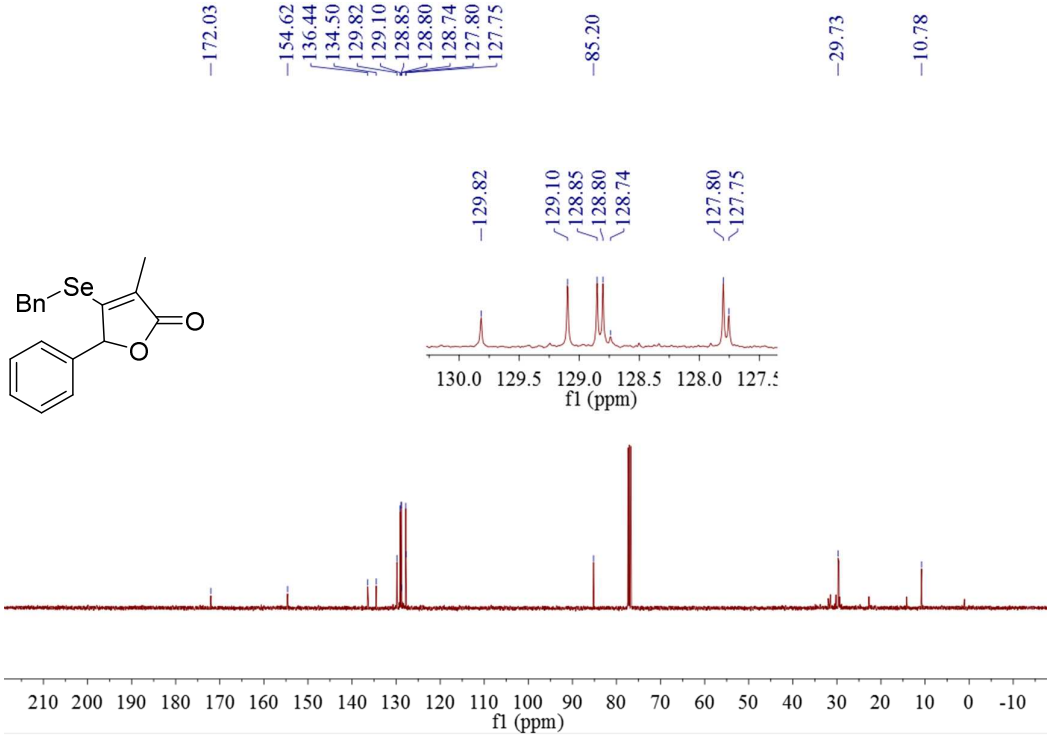
^{13}C NMR spectrum of **4h** in $CDCl_3$



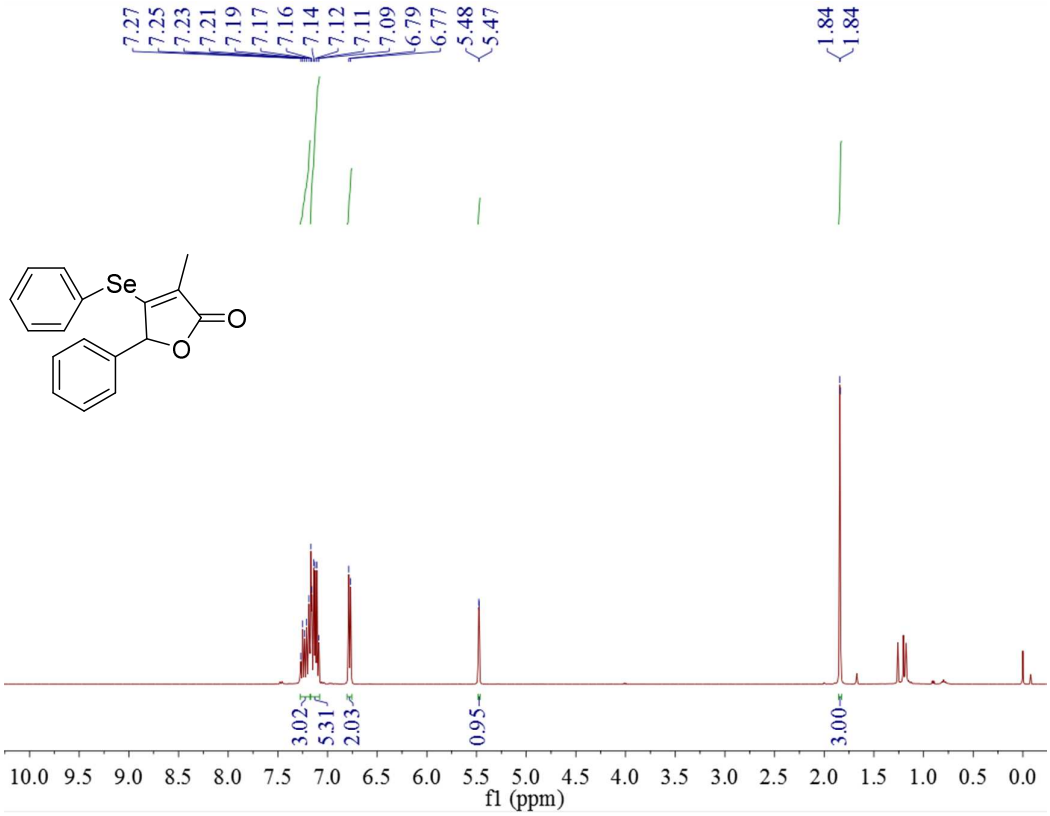
^{1}H NMR spectrum of **6a** in $CDCl_3$



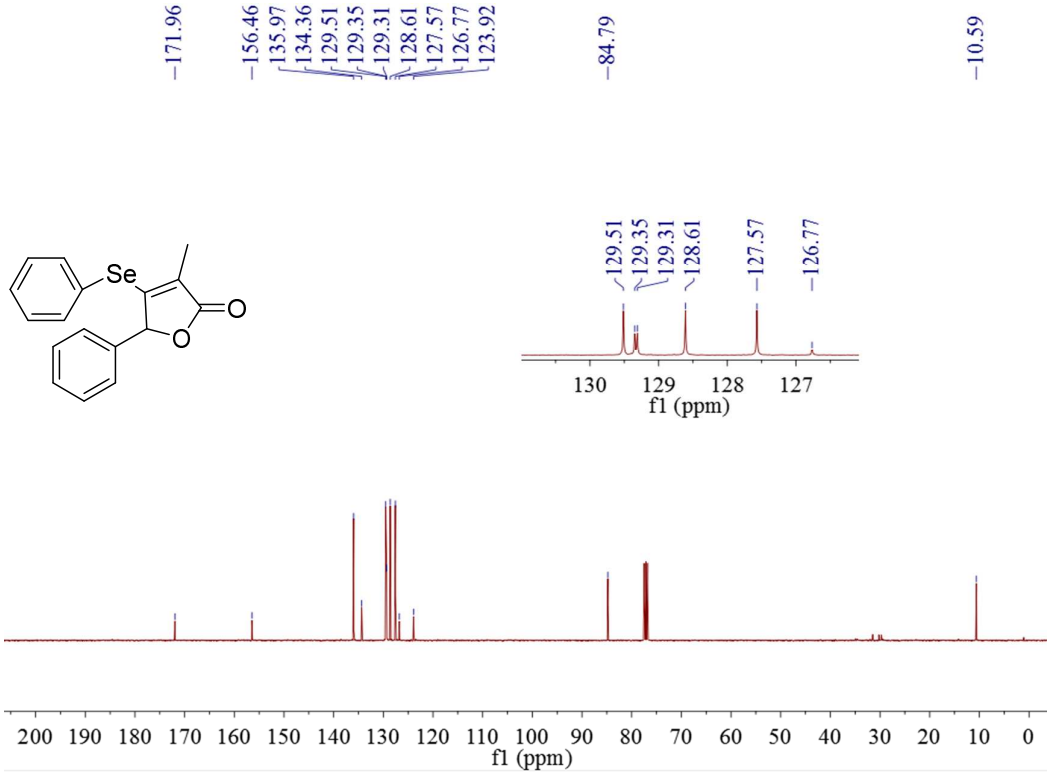
^{13}C NMR spectrum of **6a** in $CDCl_3$



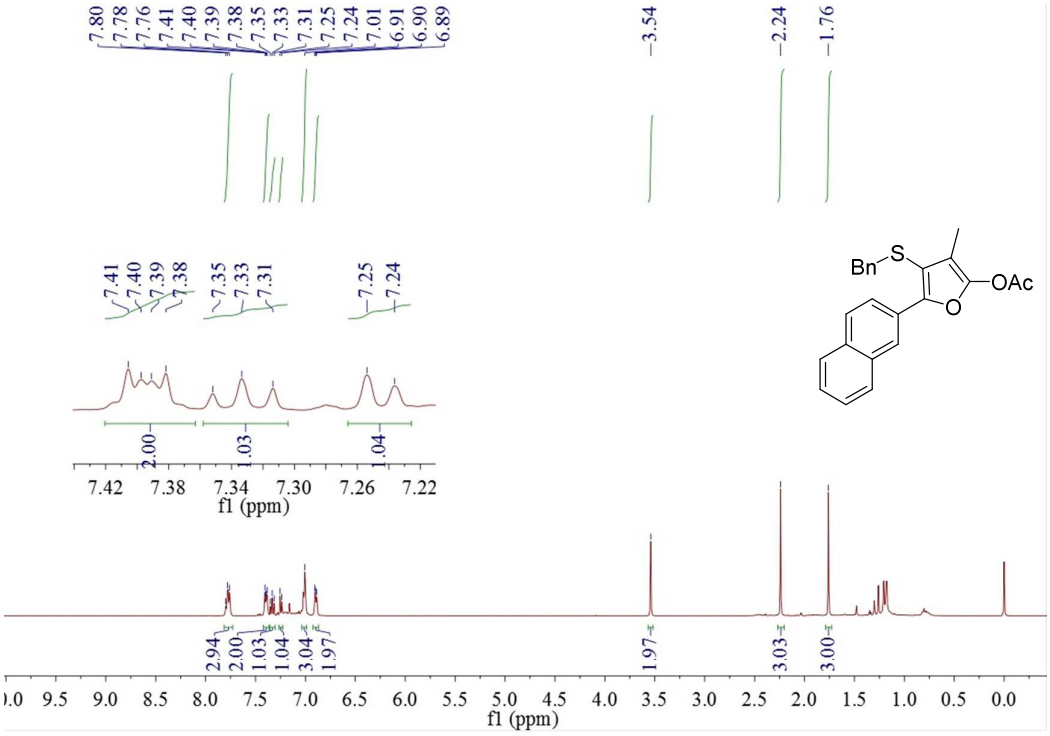
^{1}H NMR spectrum of **6b** in $CDCl_3$



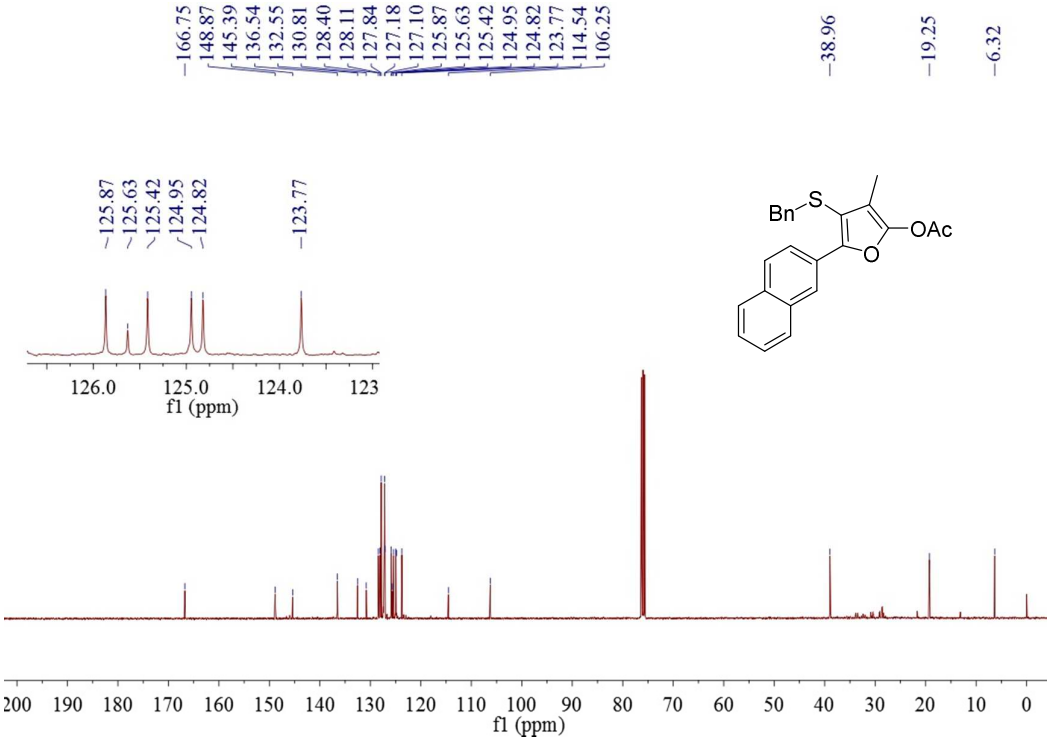
^{13}C NMR spectrum of **6b** in $CDCl_3$



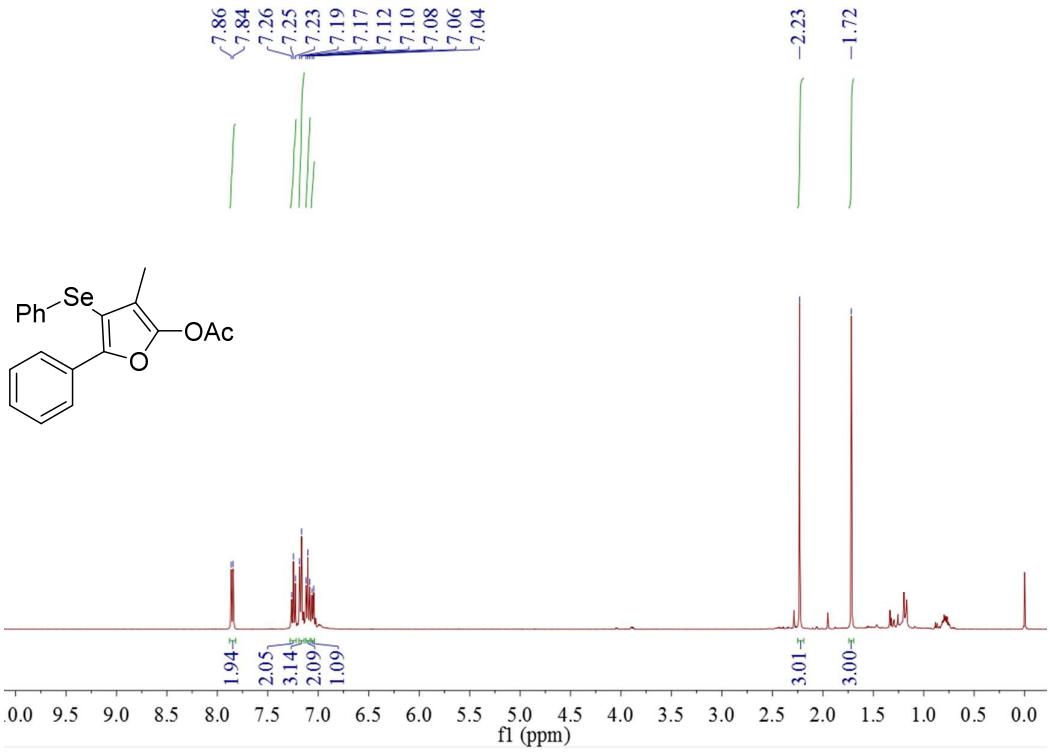
^{1}H NMR spectrum of **7** in $CDCl_3$



^{13}C NMR spectrum of **7** in $CDCl_3$



^{1}H NMR spectrum of **8** in $CDCl_3$



^{13}C NMR spectrum of **8** in $CDCl_3$