

## **SUPPORTING INFORMATION**

### **Application of *N*-acylbenzotriazoles in the synthesis of 5-substituted-2-ethoxy-1,3,4-oxadiazoles as building blocks toward 3,5-disubstituted 1,3,4-oxadiazole-2(3H)-ones**

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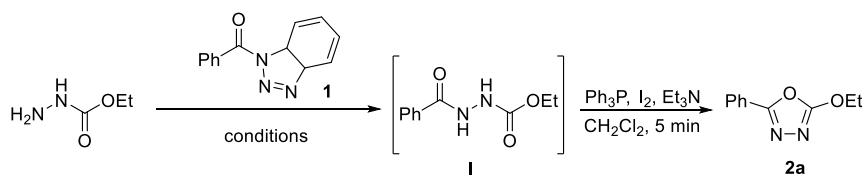
<sup>a</sup>Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science,  
Chiang Mai University, Chiang Mai 50200, Thailand

<sup>b</sup>Graduate School, Chiang Mai University, Chiang Mai 50200, Thailand

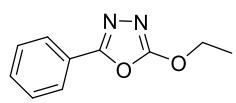
<sup>c</sup>Center of Excellence in Materials Science and Technology, Chiang Mai University, Chiang Mai  
50200, Thailand

Email: [mookdap55@gmail.com](mailto:mookdap55@gmail.com)

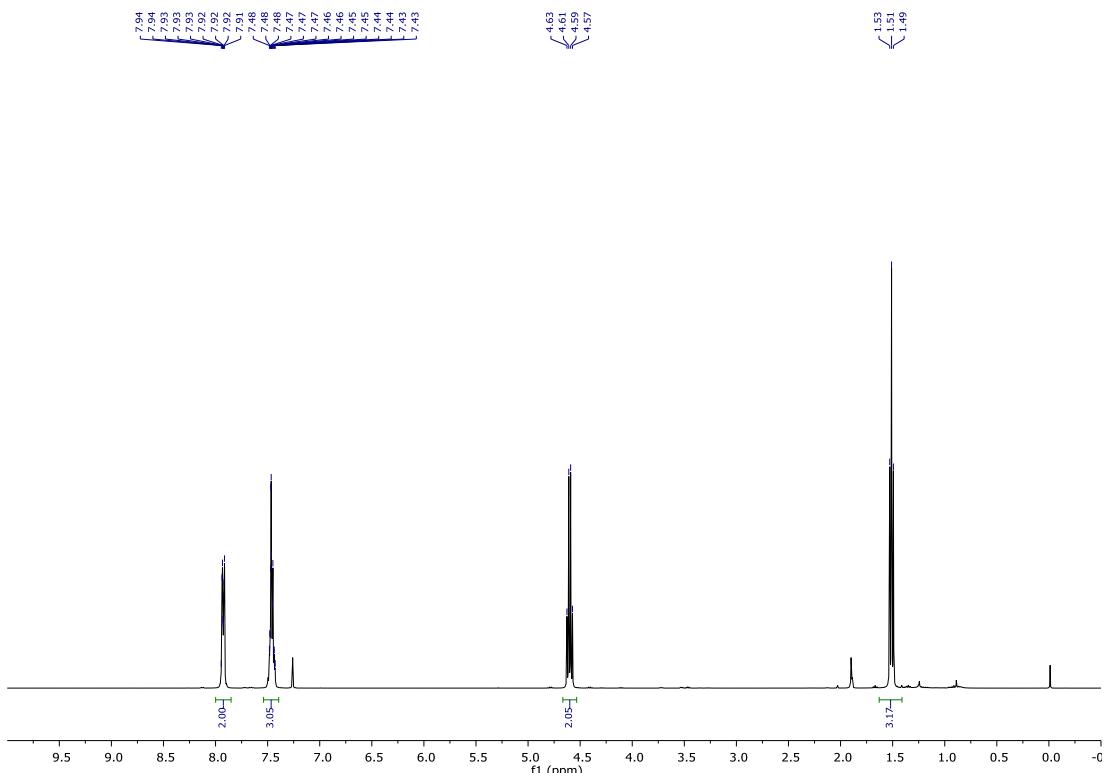
**Table S1** Optimization of the reaction conditions



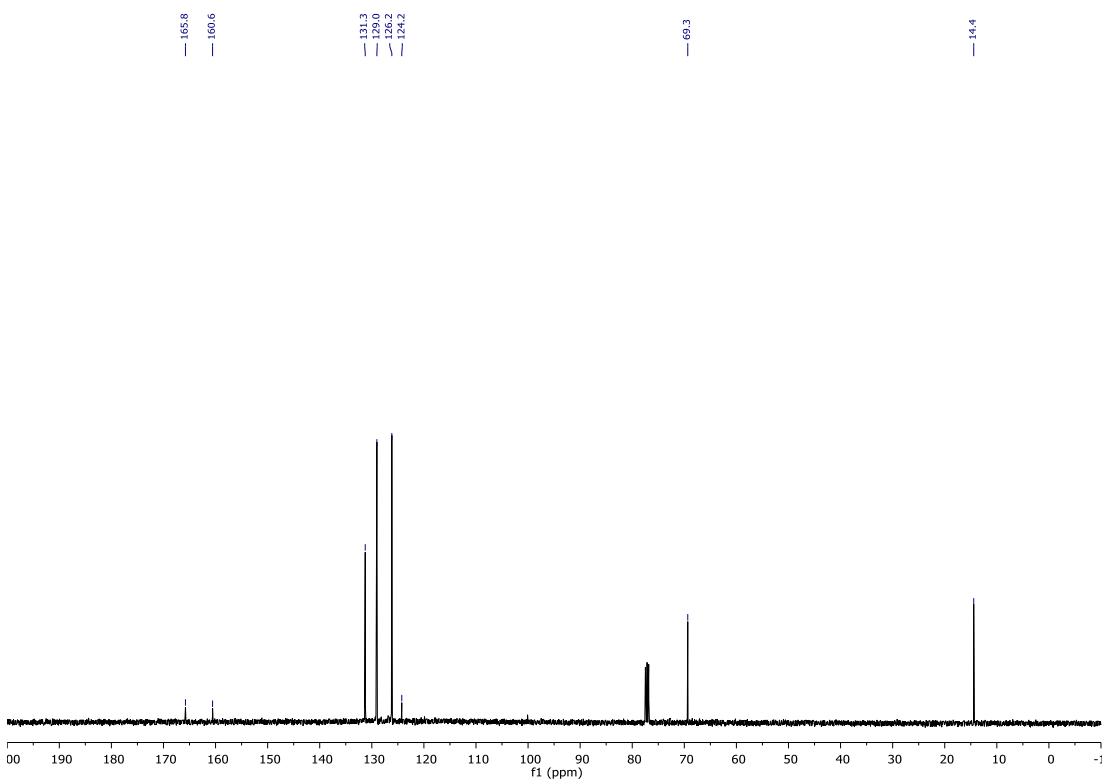
Entry	Conditions	Yield of <b>I</b> (%)	Yield of <b>2a</b> (%)
1	No base, CH <sub>2</sub> Cl <sub>2</sub> , sonication, 25 °C, 30 min	40	-
2	Et <sub>3</sub> N, CH <sub>2</sub> Cl <sub>2</sub> , sonication, 25 °C, 30 min	quant.	NR
3	K <sub>2</sub> CO <sub>3</sub> , CH <sub>2</sub> Cl <sub>2</sub> , sonication, 25 °C, 30 min	quant.	85
4	K <sub>2</sub> CO <sub>3</sub> , DMAP, CH <sub>2</sub> Cl <sub>2</sub> , sonication, 25 °C, 10 min	quant.	86

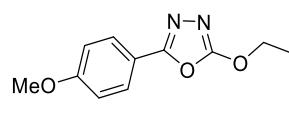


(Scheme 2, 2a); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

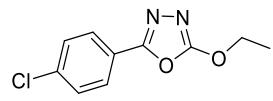
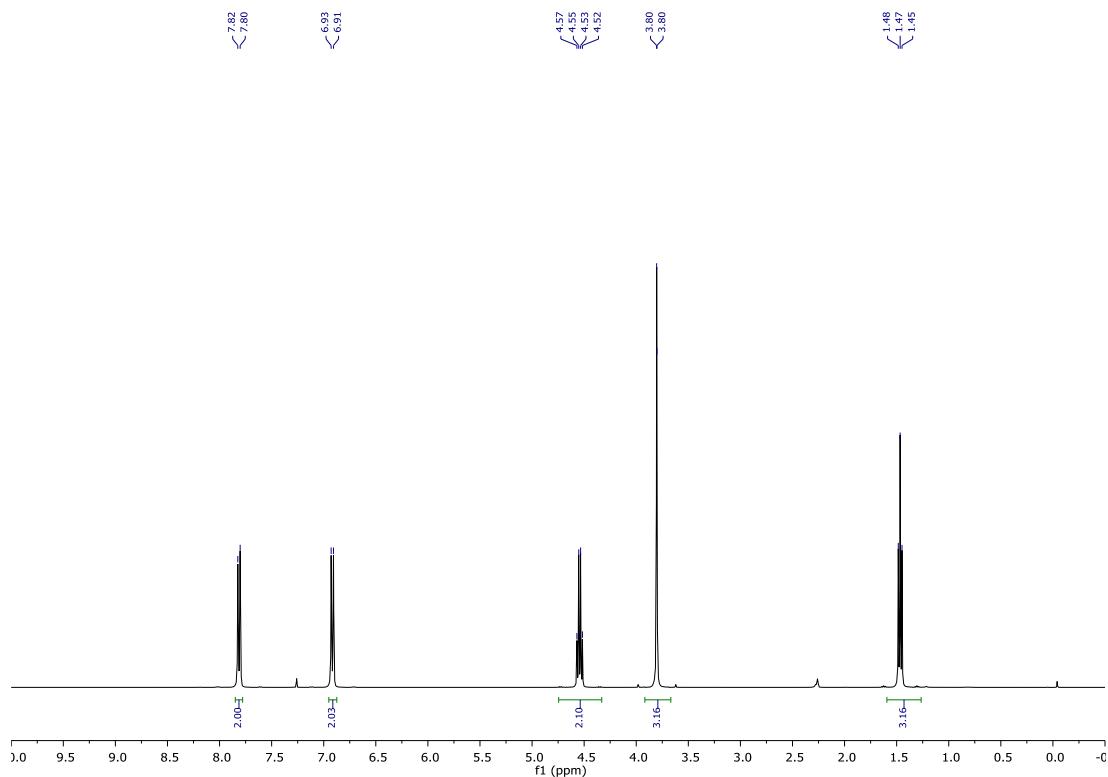


(Scheme 2, 2a); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

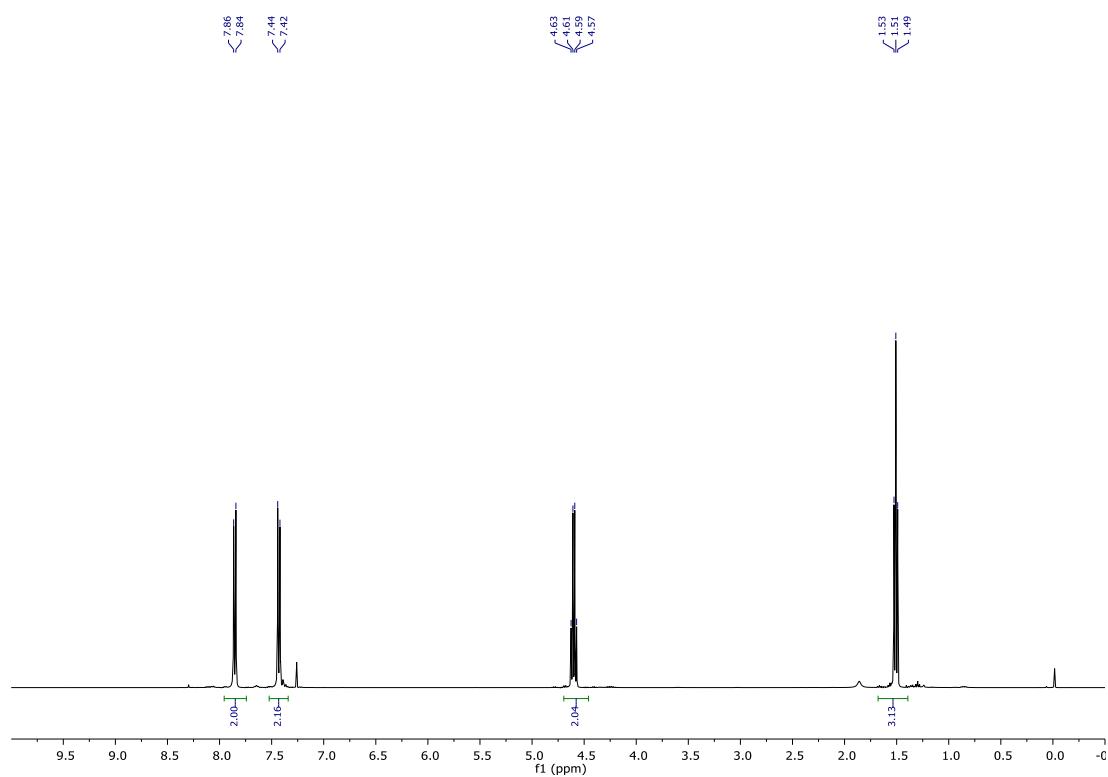


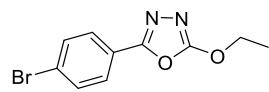


(Scheme 2, **2b**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

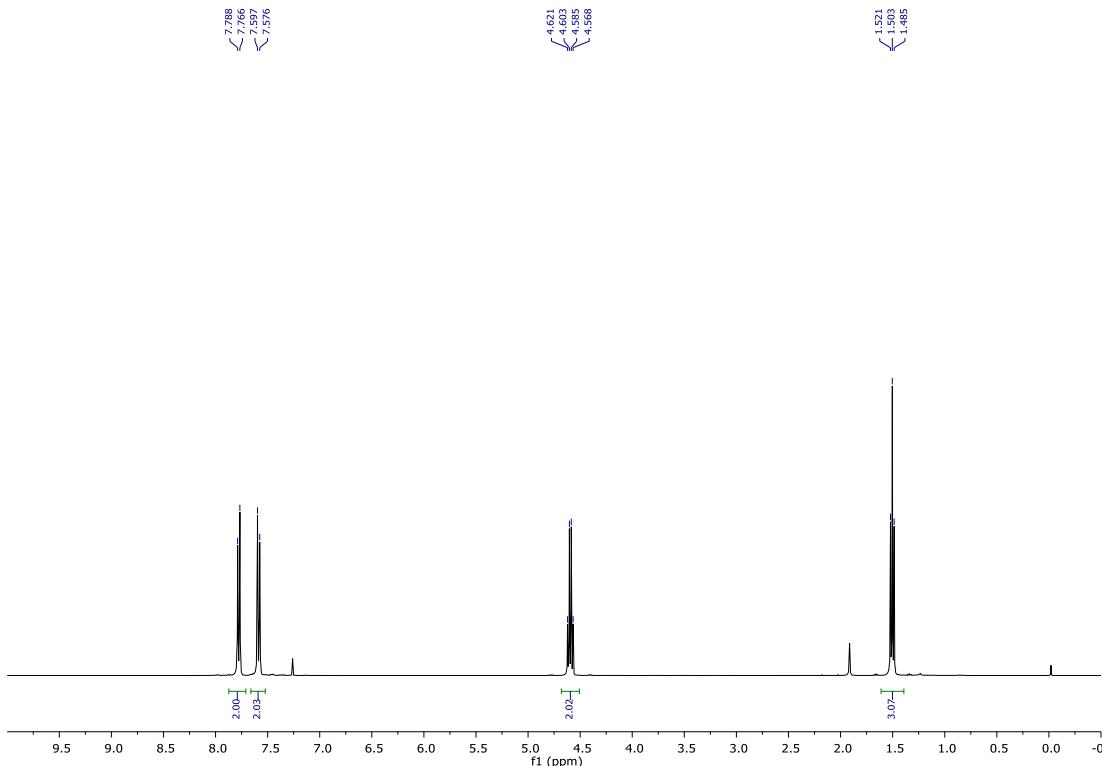


(Scheme 2, **2c**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

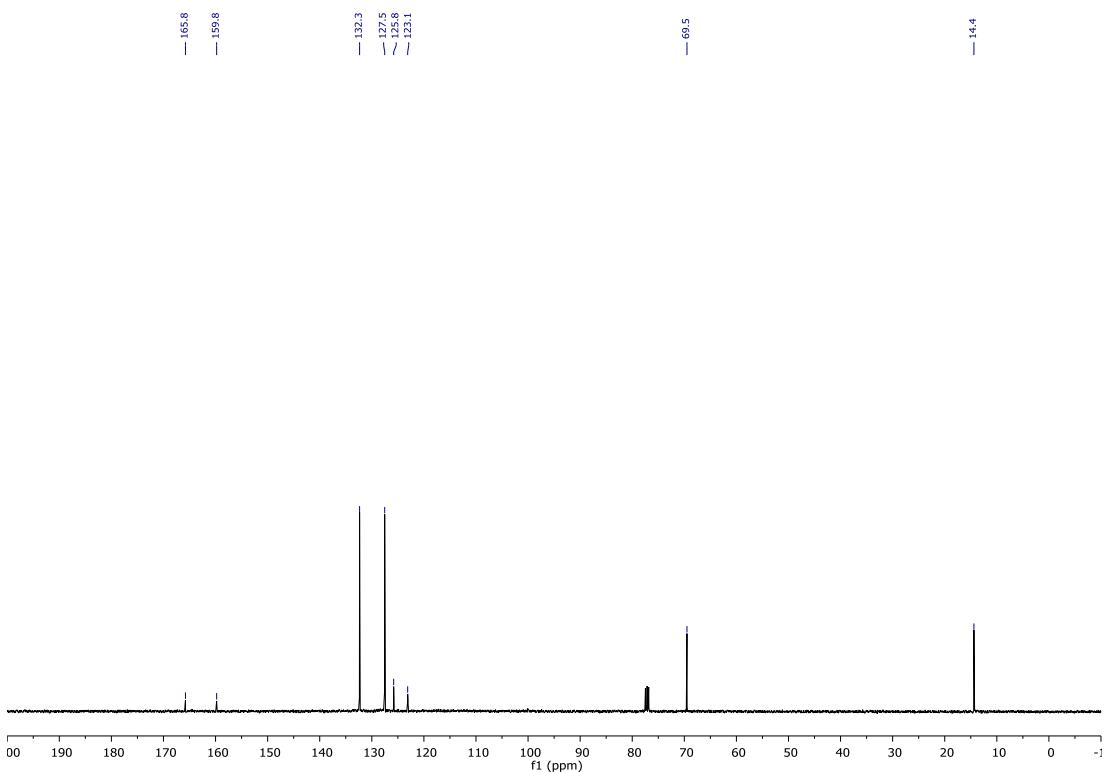


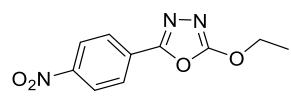


(Scheme 2, **2d**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

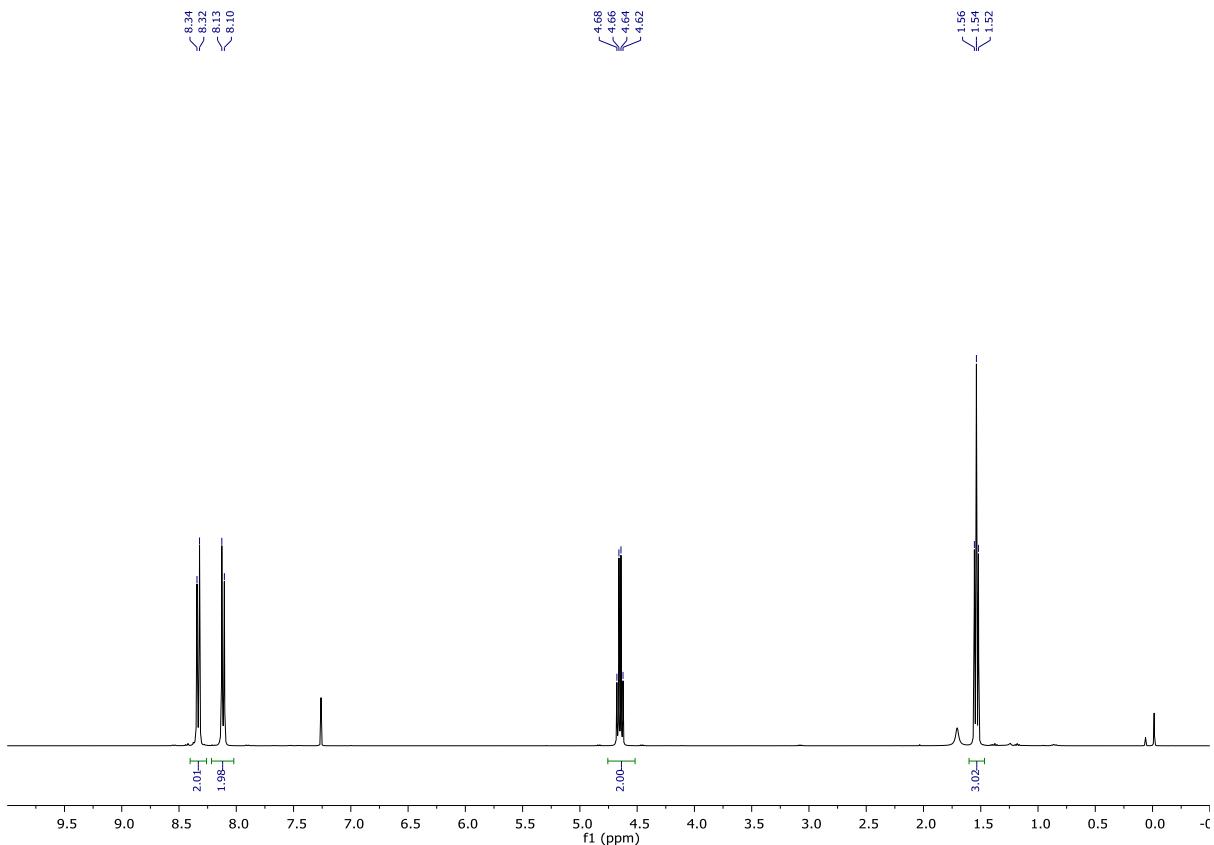


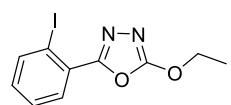
(Scheme 2, **2d**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )





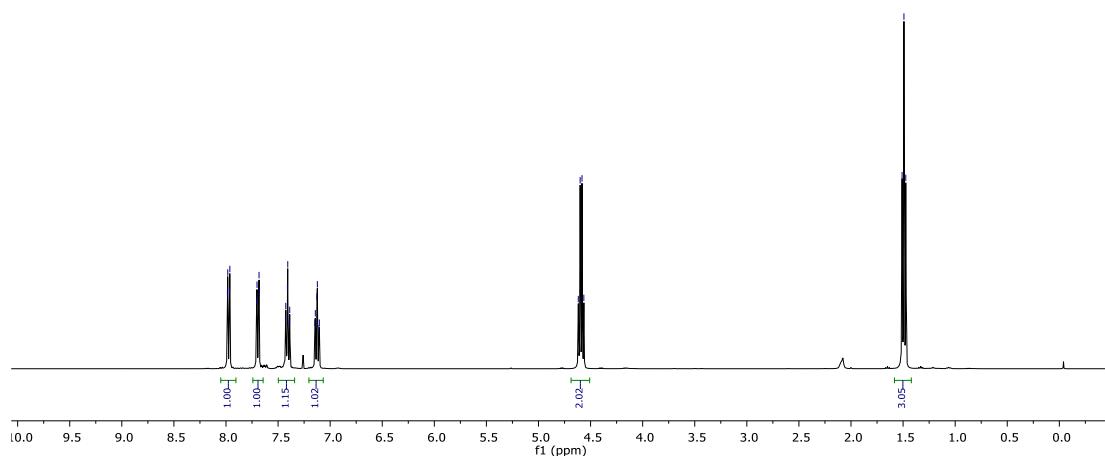
(Scheme 2, **2e**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )





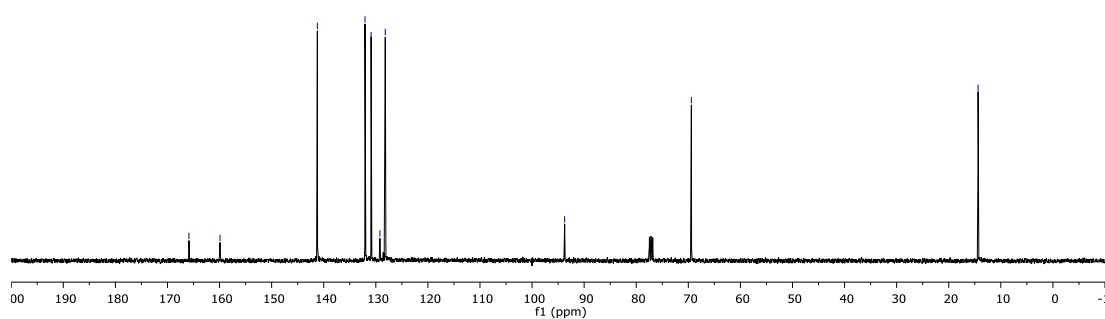
(Scheme 2, **2f**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

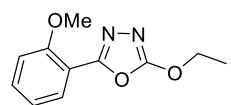
Chemical shifts ( $\delta$ ): 7.99, 7.98, 7.97, 7.96, 7.95, 7.71, 7.70, 7.69, 7.68, 7.43, 7.41, 7.41, 7.39, 7.39, 7.39, 7.15, 7.14, 7.14, 7.12, 7.11, 7.10, 4.62, 4.60, 4.58, 4.56, 1.51, 1.49, 1.47 ppm.



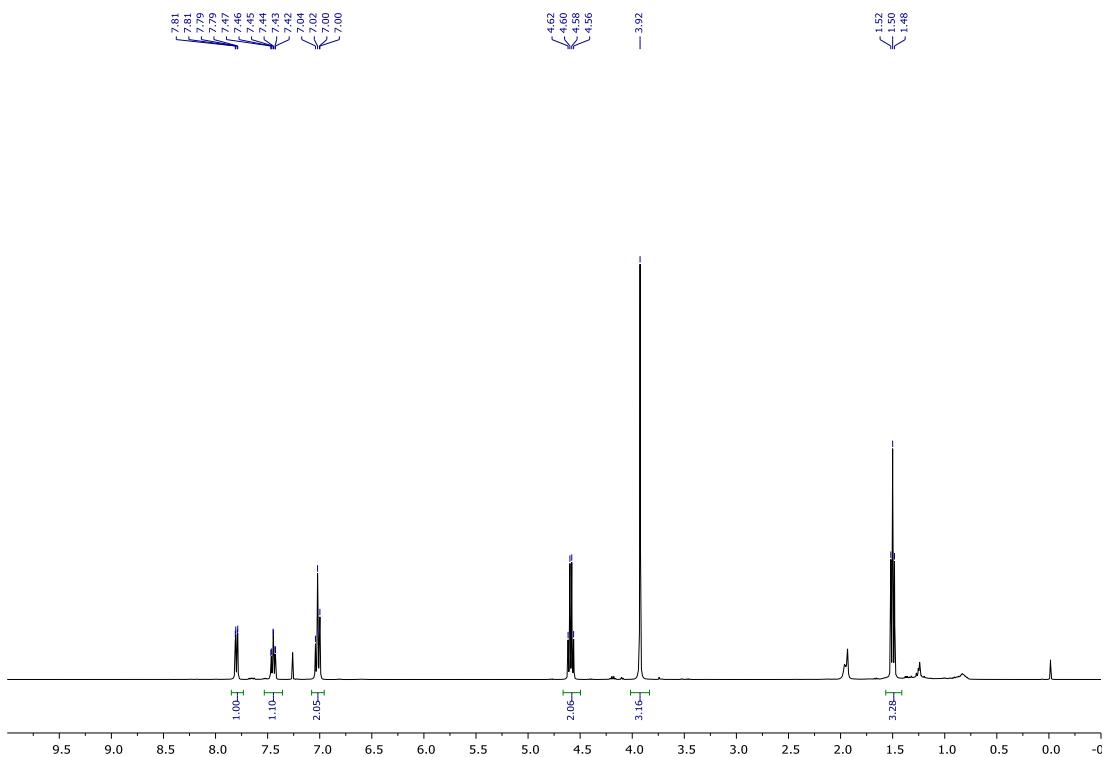
(Scheme 2, **2f**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

Chemical shifts ( $\delta$ ): 165.9, 159.9, 141.2, 132.1, 132.0, 128.2, 93.7, 69.4, 14.4 ppm.

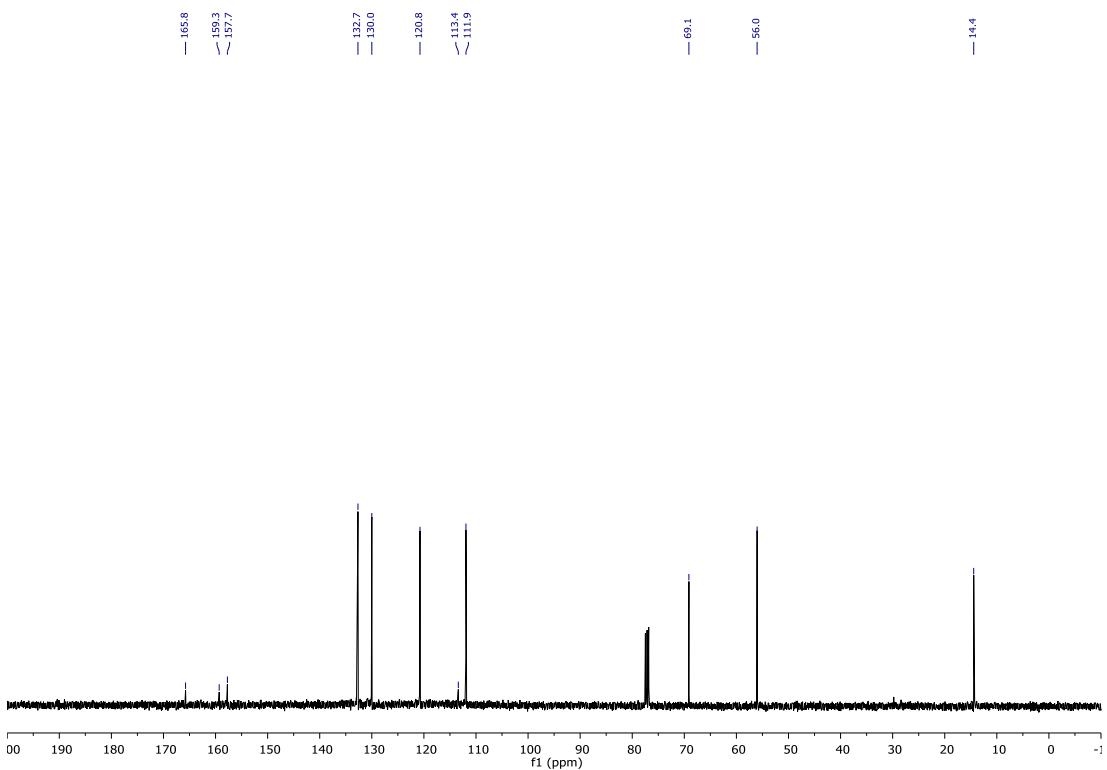


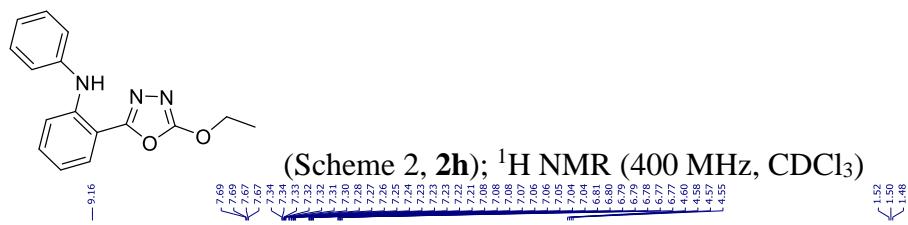


(Scheme 2, 2g);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

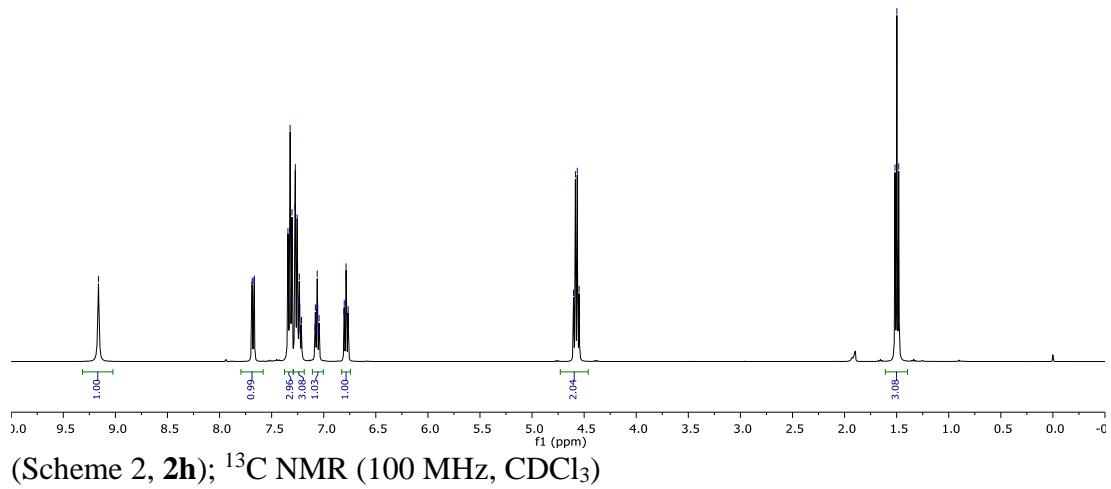


(Scheme 2, 2g);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

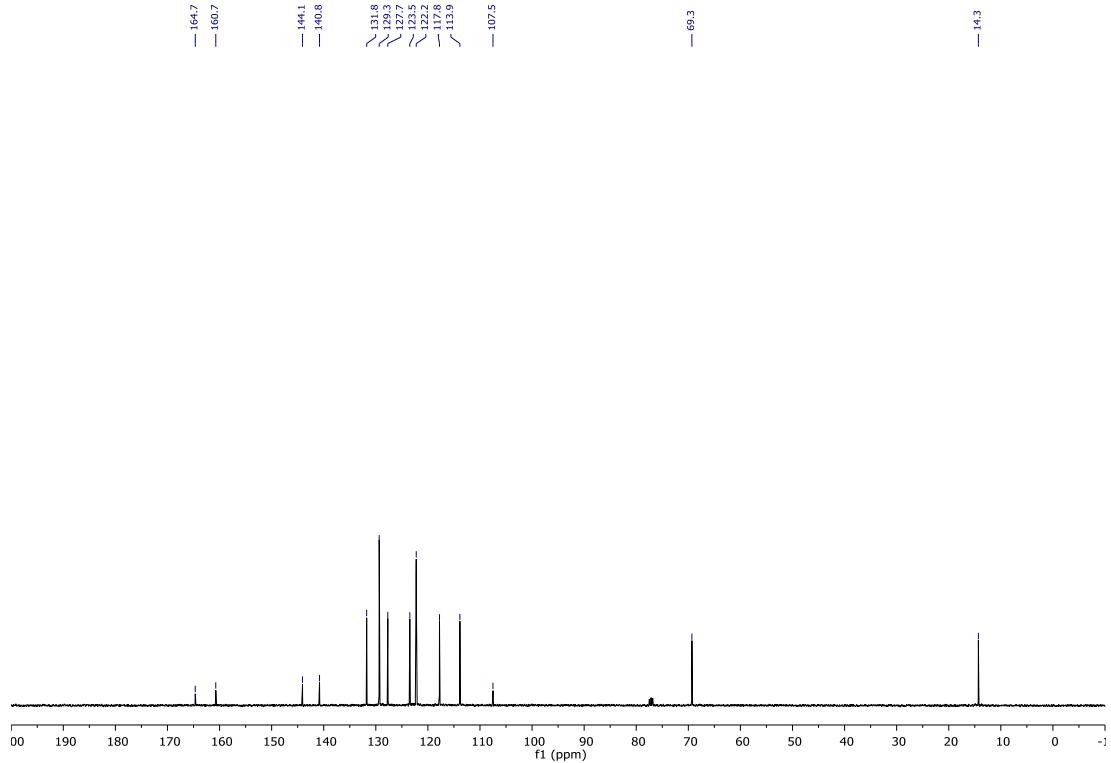


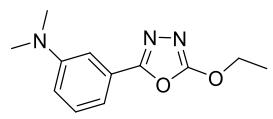


(Scheme 2, **2h**); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

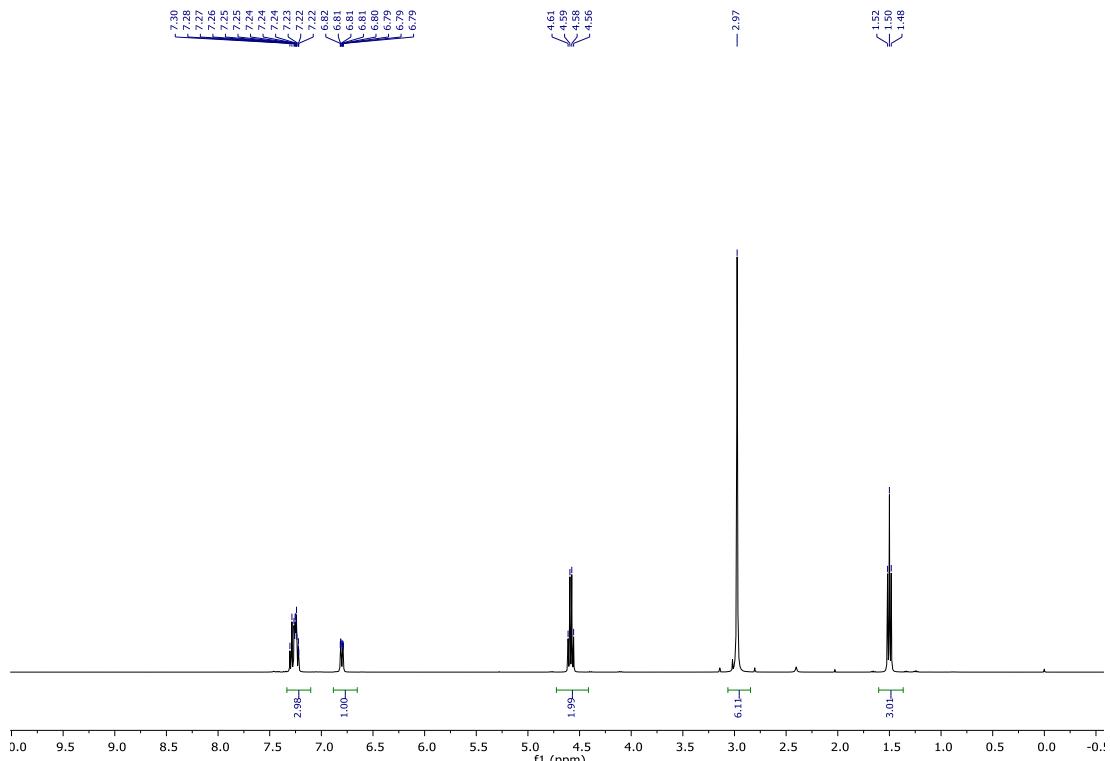


(Scheme 2, **2h**); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

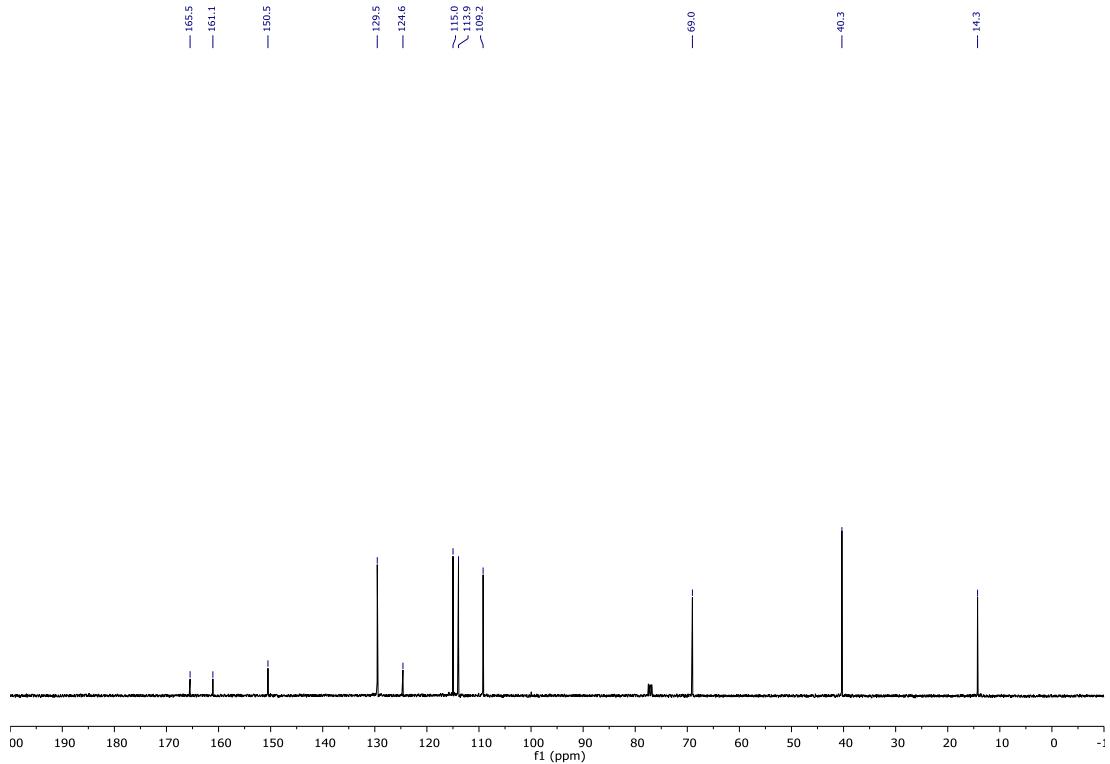


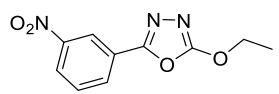


(Scheme 2, **2i**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

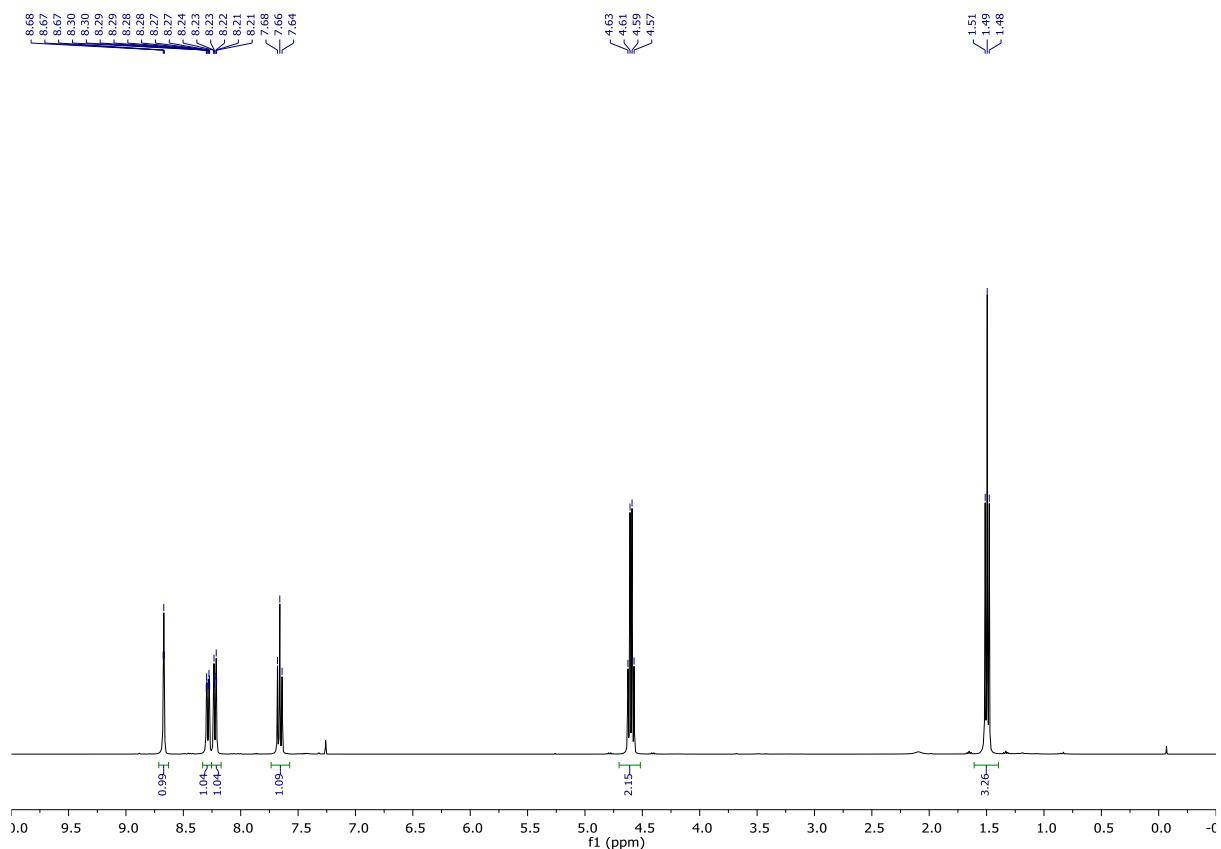


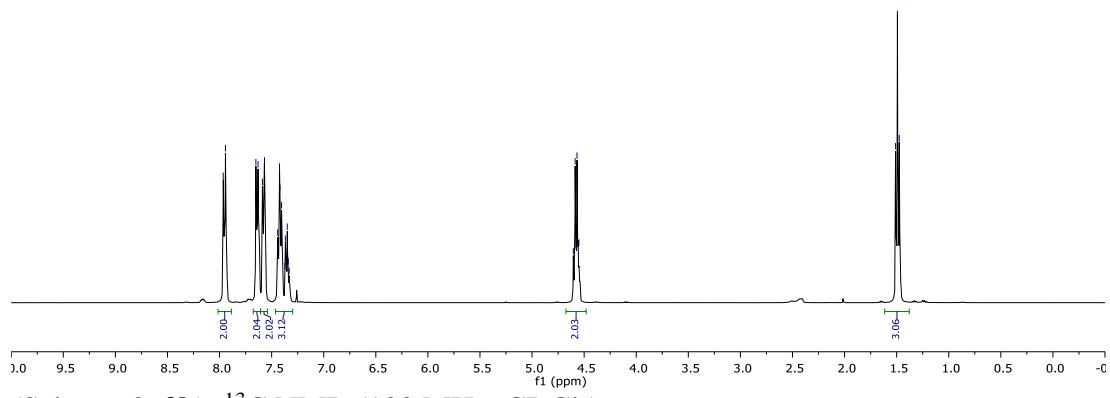
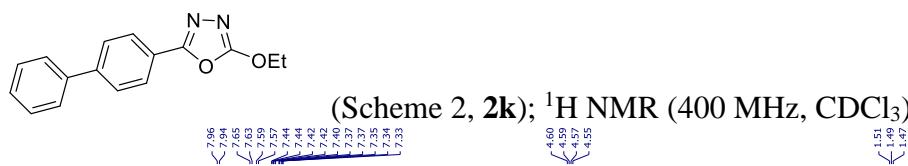
(Scheme 2, **2i**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )





(Scheme 2, **2j**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

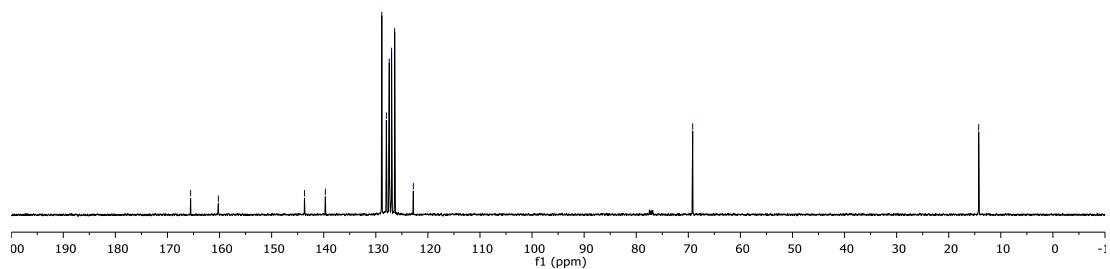


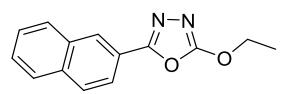


**(Scheme 2, 2k);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )**

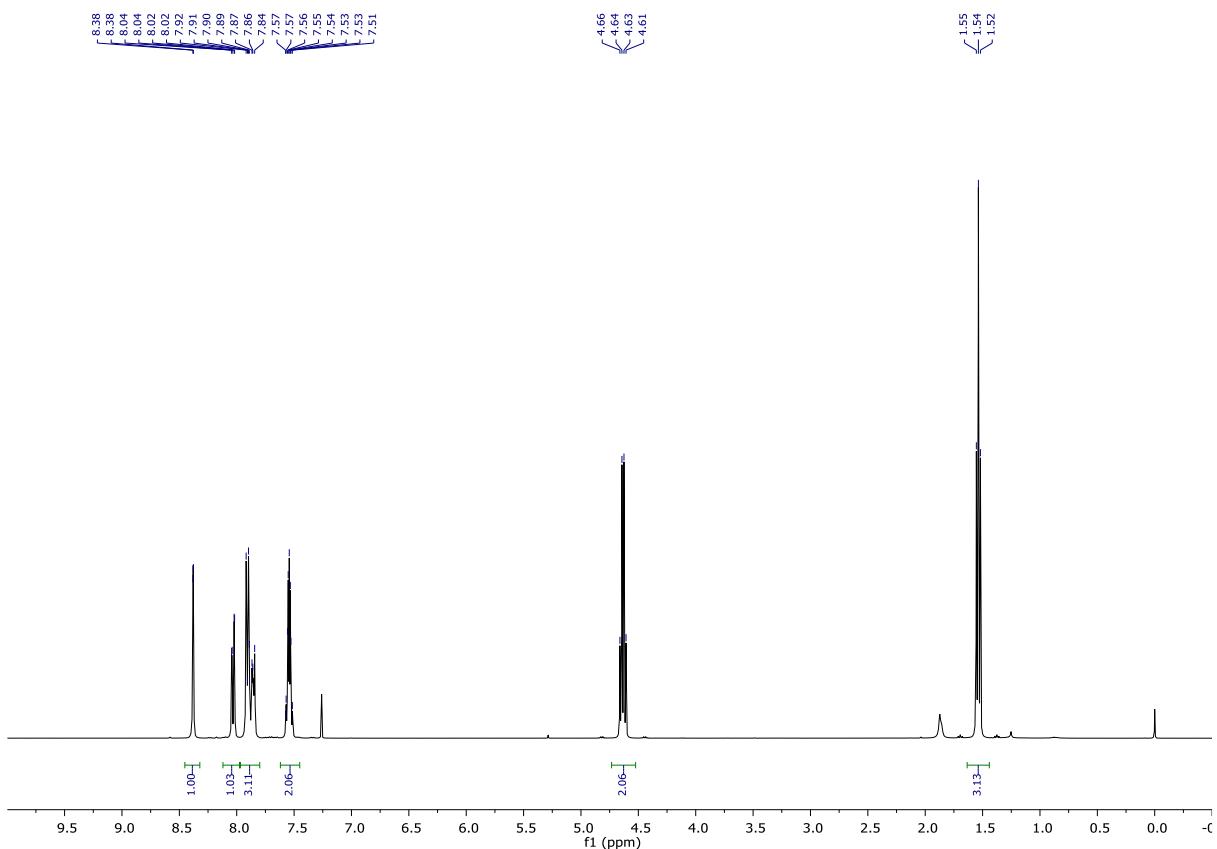
$^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CDCl}_3$ ) showing chemical shifts ( $\delta$ ) in ppm. Key peaks are labeled with their chemical shifts:

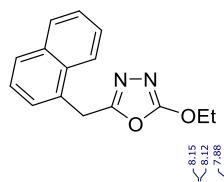
- 165.6, 160.2, 143.7, 139.7
- 128.9, 128.0, 127.4, 127.0, 126.4, 122.8
- 69.2, 14.3



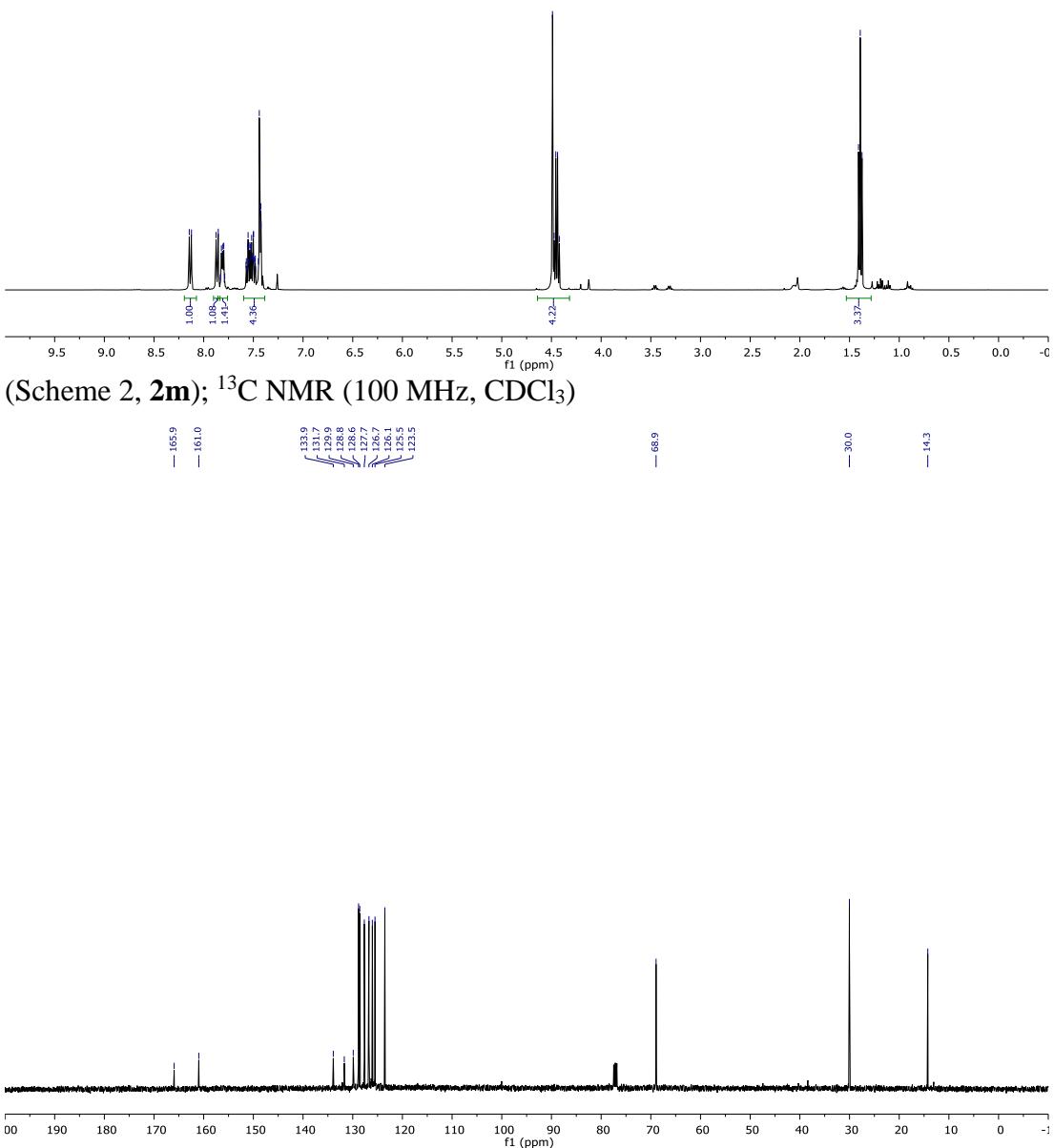


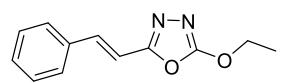
(Scheme 2, **2l**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



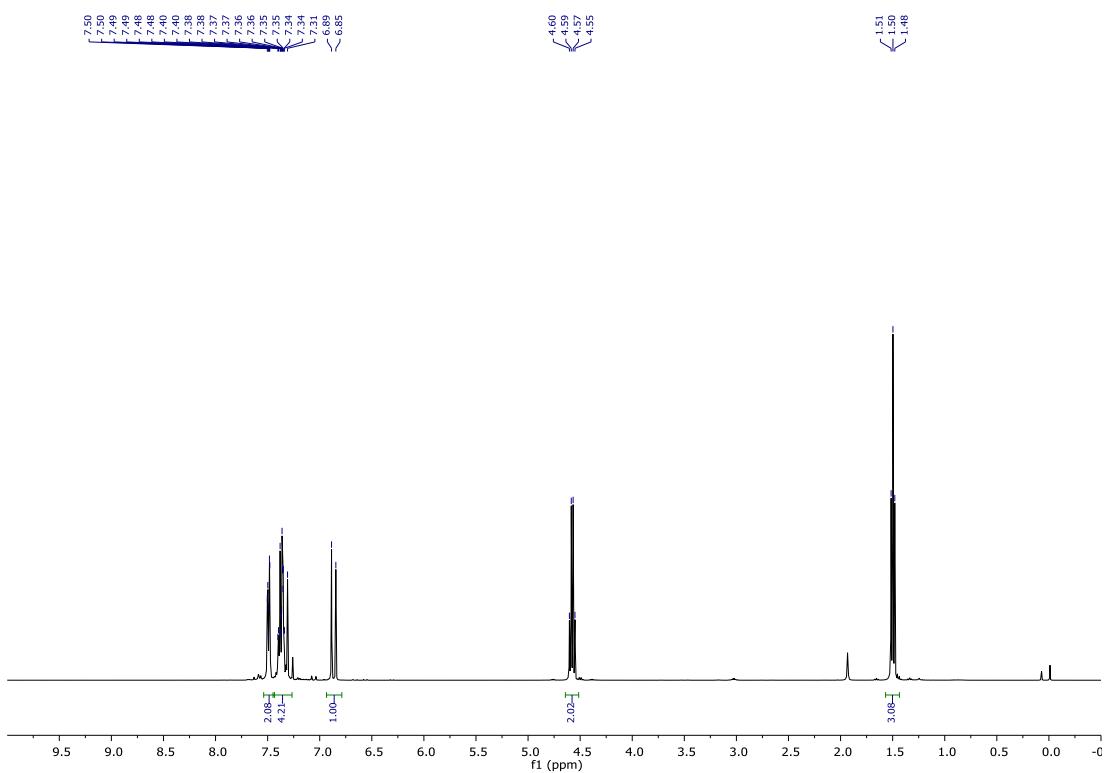


(Scheme 2, **2m**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

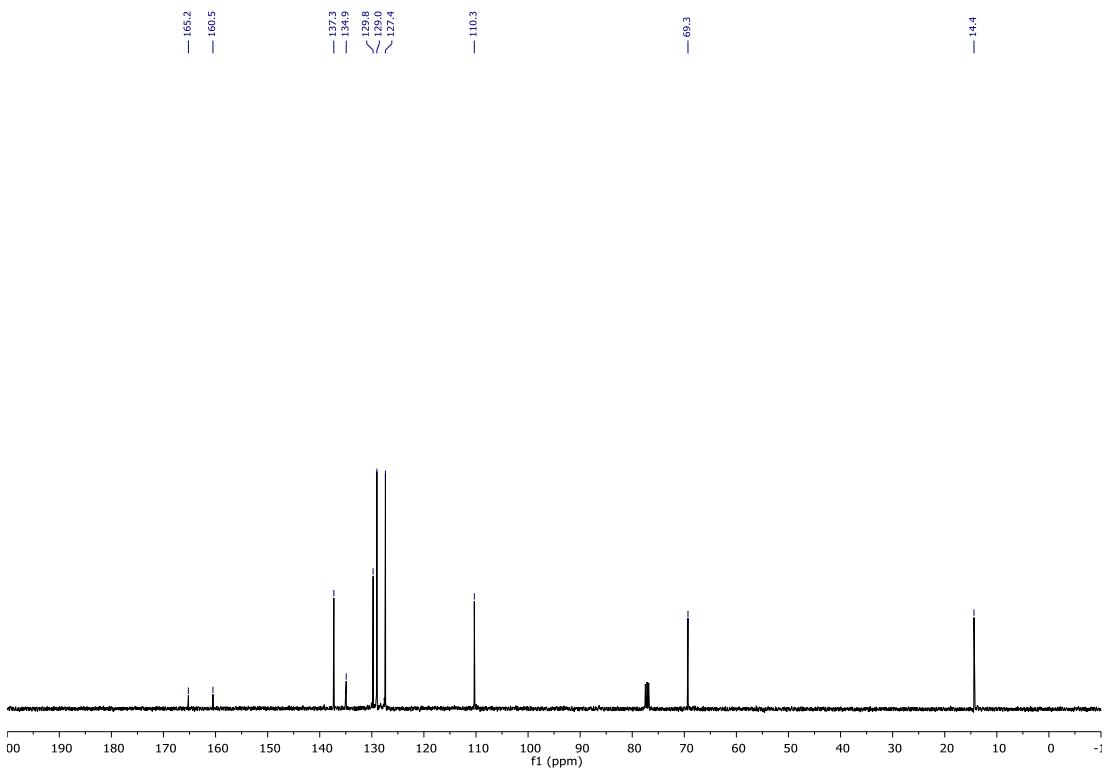


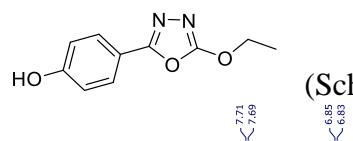


(Scheme 2, **2n**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

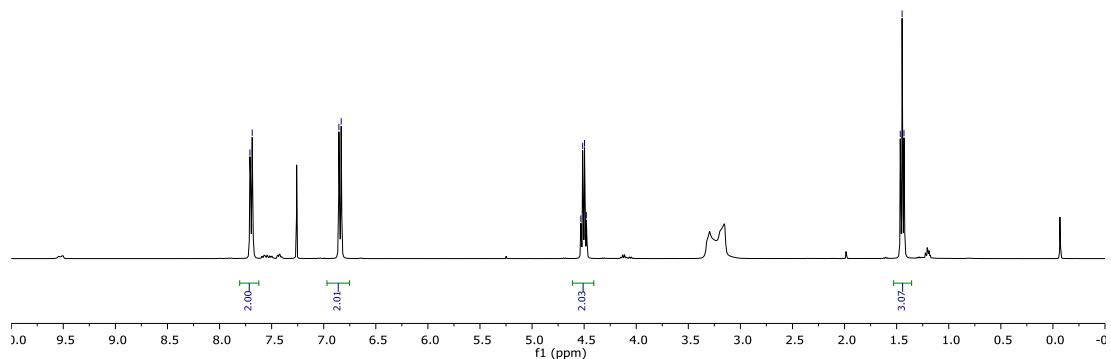


(Scheme 2, **2n**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

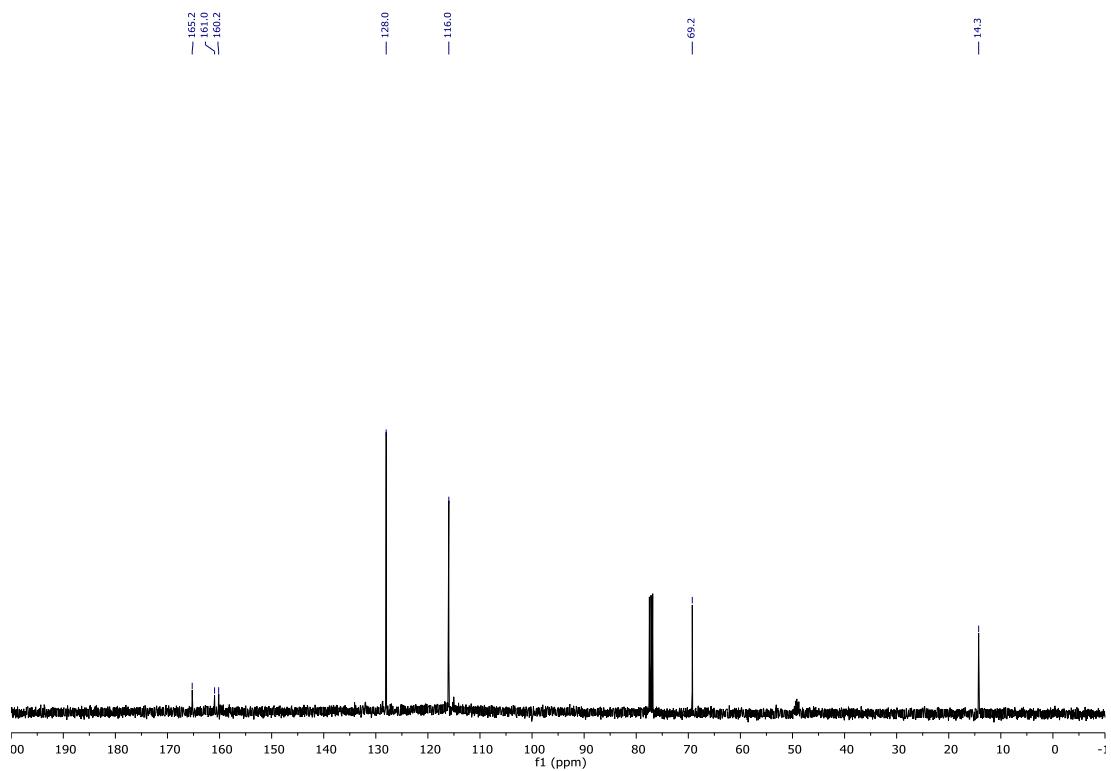


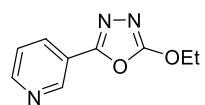


(Scheme 2, **2o**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3 + \text{CD}_3\text{OD}$  3 drops)

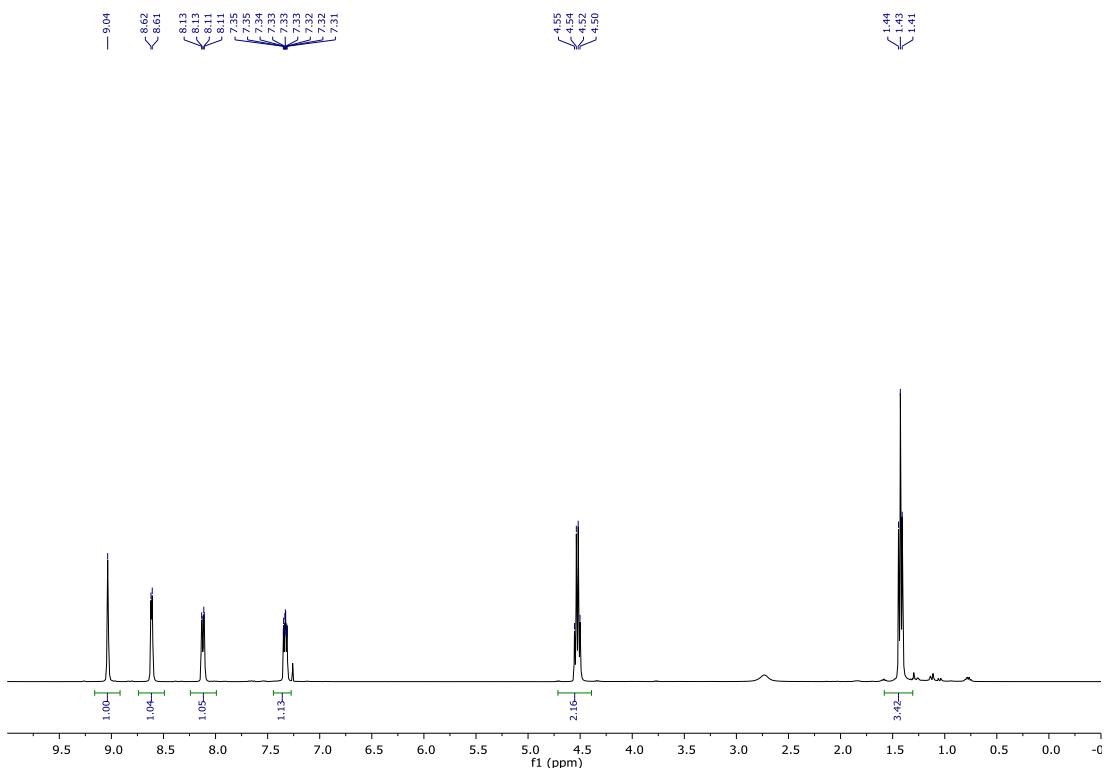


(Scheme 2, **2o**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3 + \text{CD}_3\text{OD}$  3 drops)

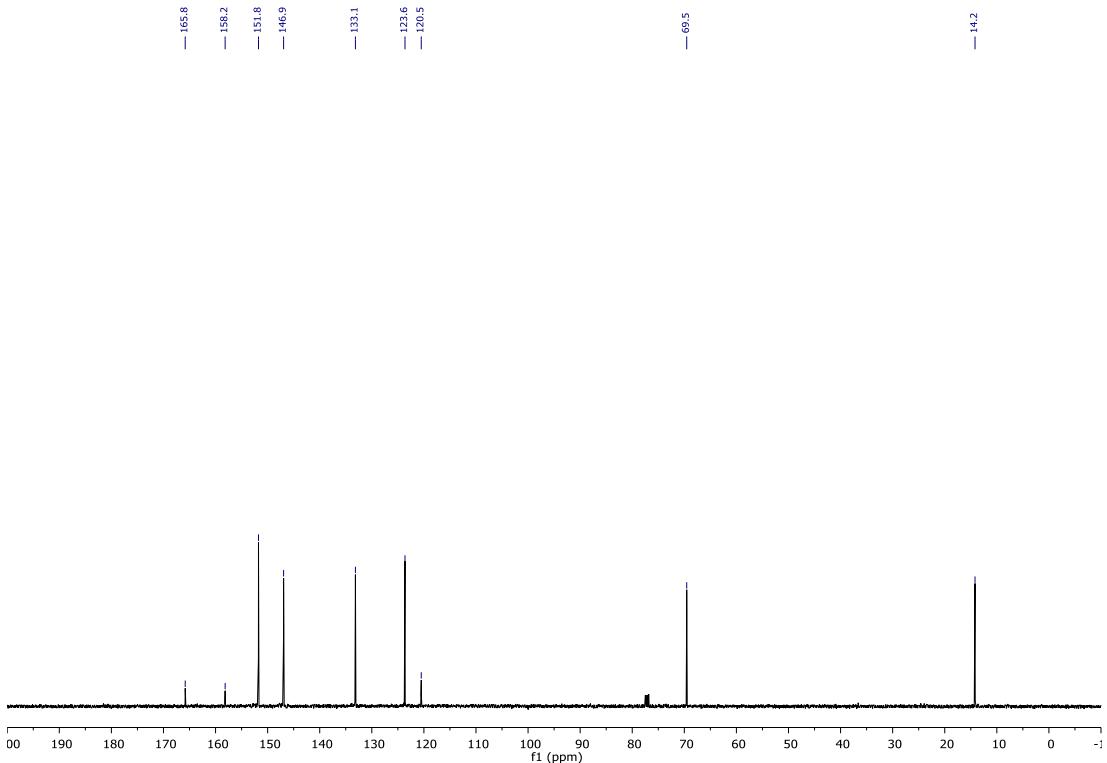


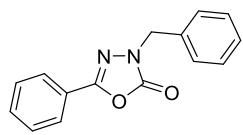


(Scheme 2, **2p**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

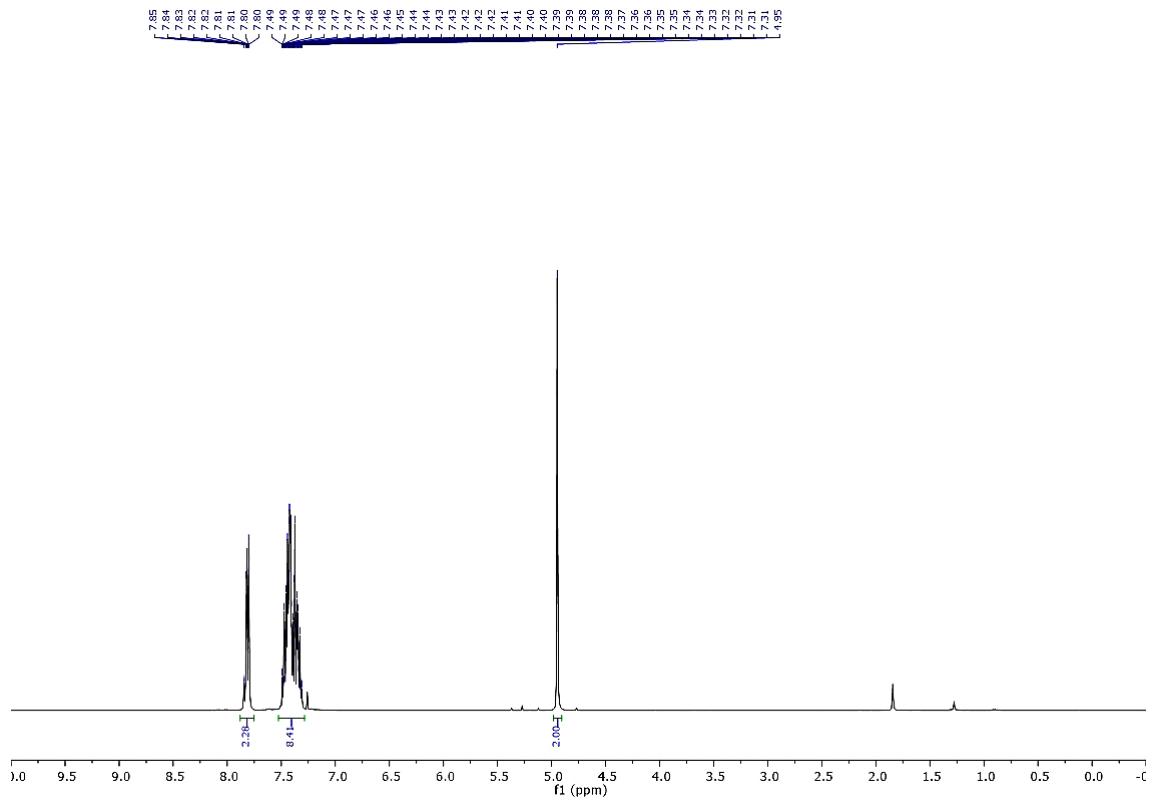


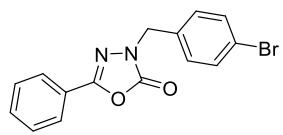
(Scheme 2, **2p**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )



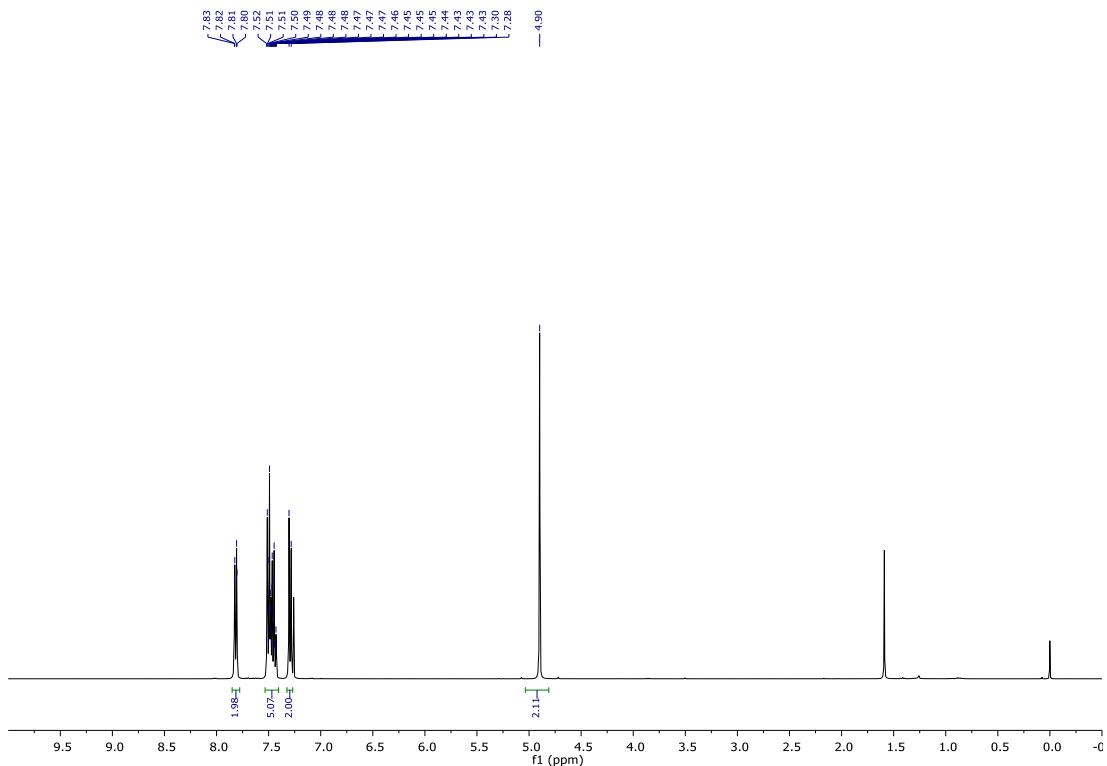


(Scheme 3, **3a**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

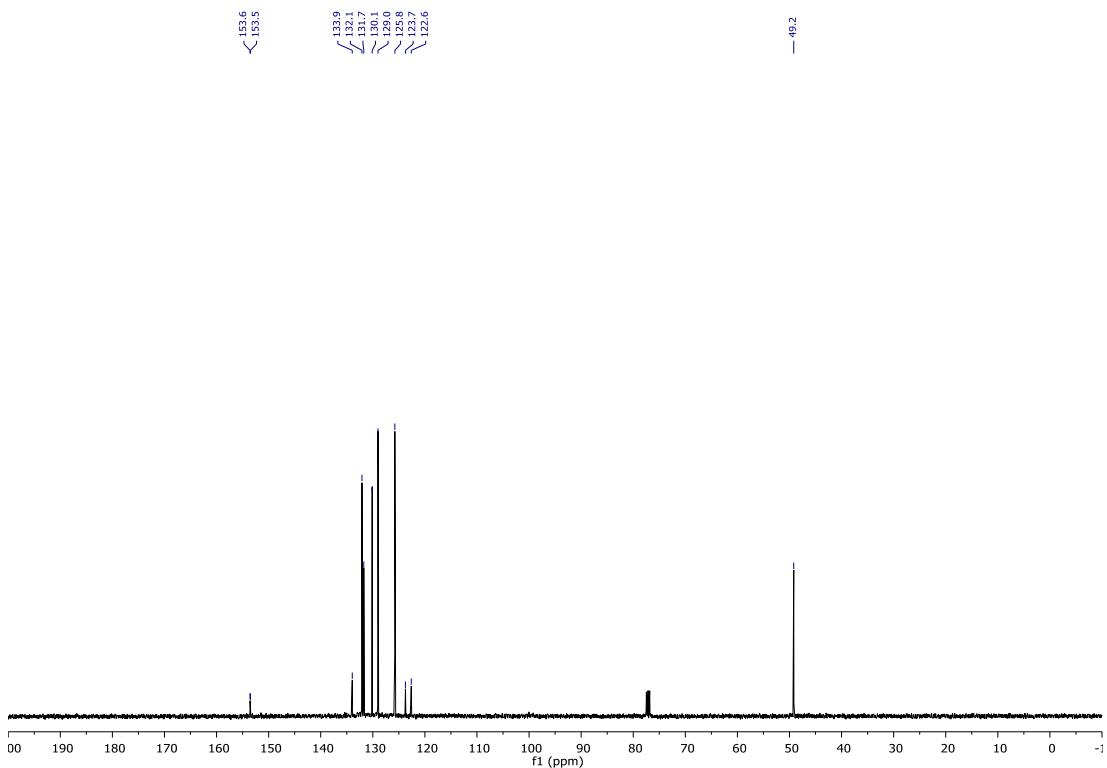


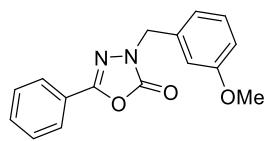


(Scheme 3, **3b**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

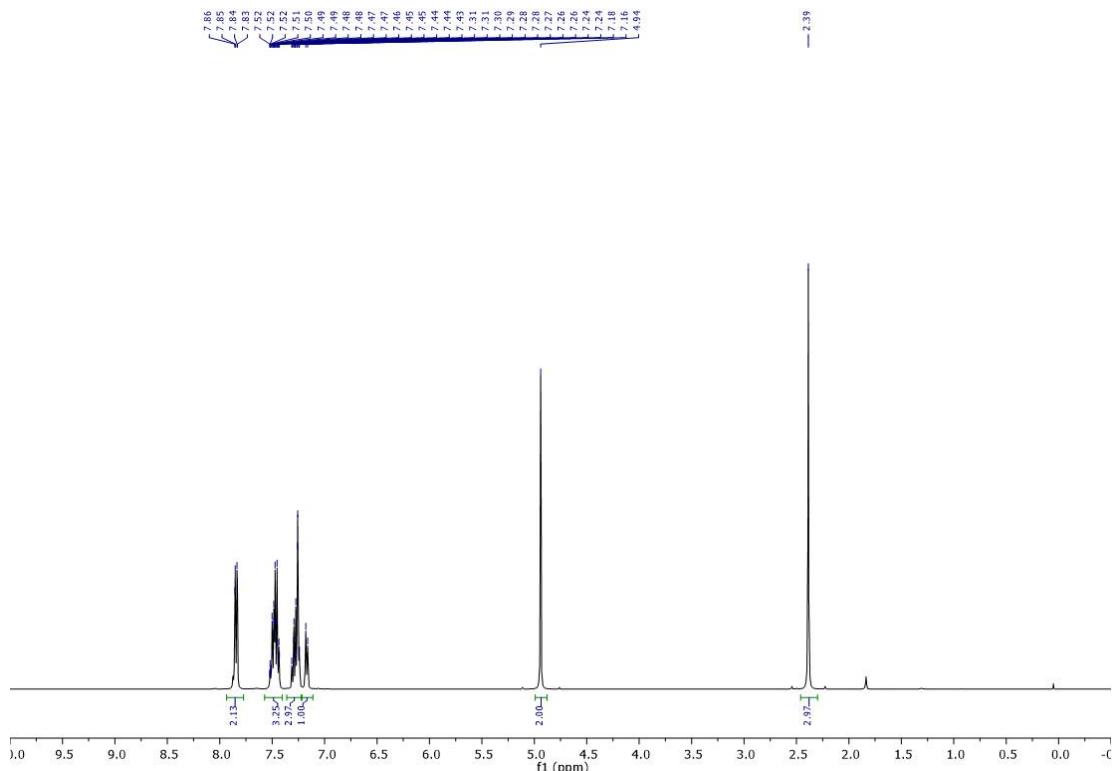


(Scheme 3, **3b**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

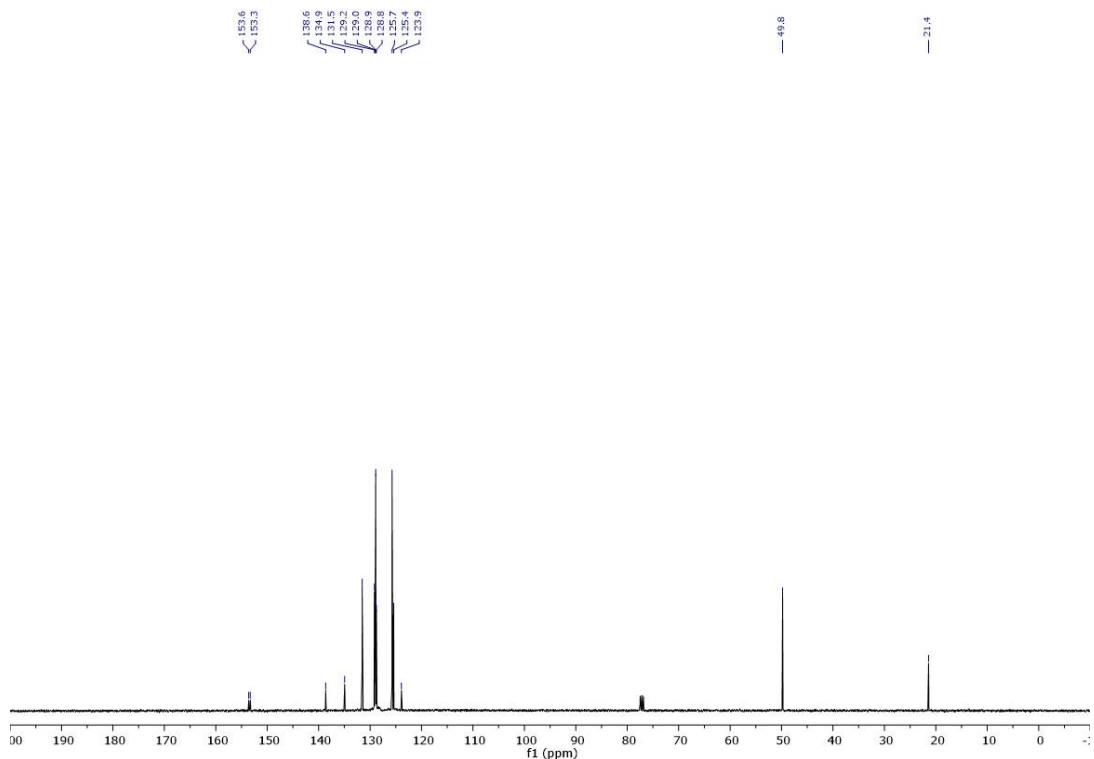


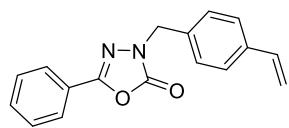


(Scheme 3, **3c**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

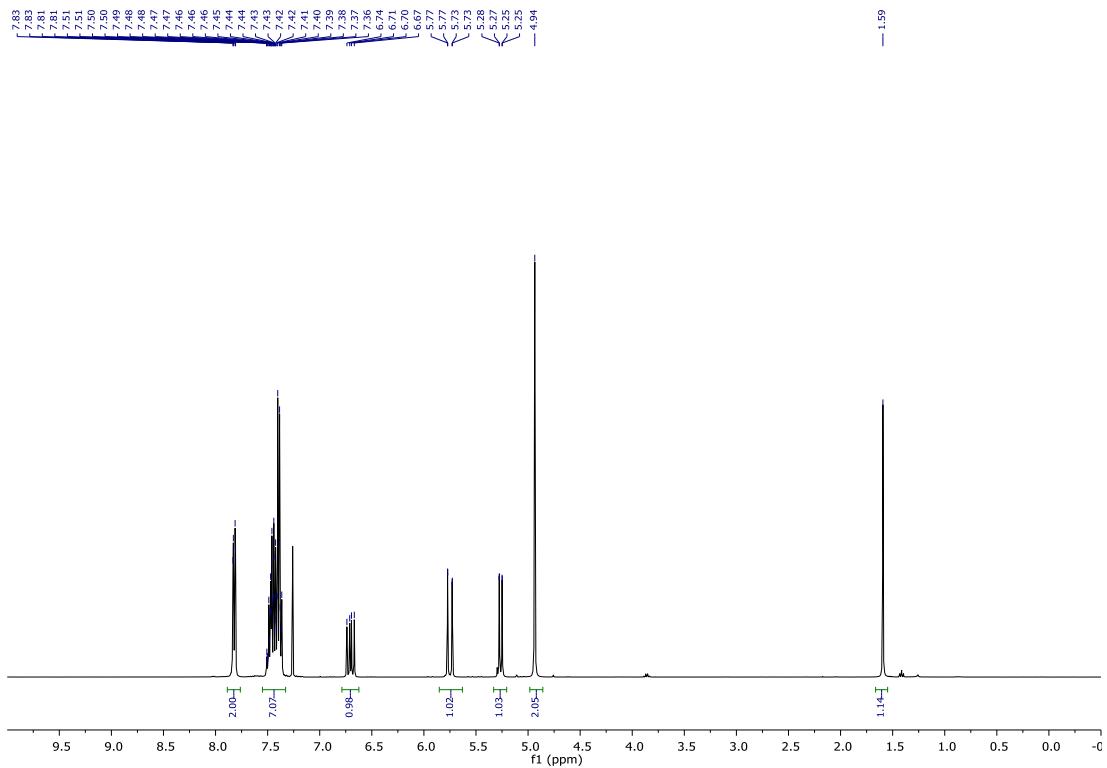


(Scheme 3, **3c**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

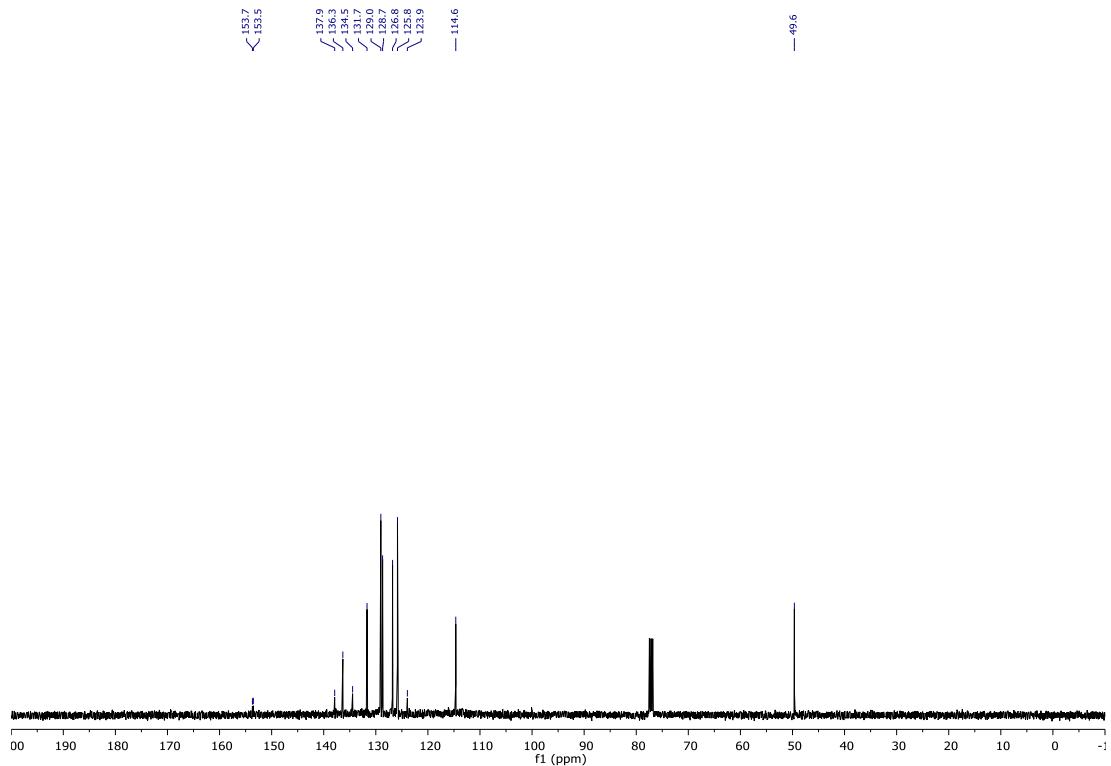


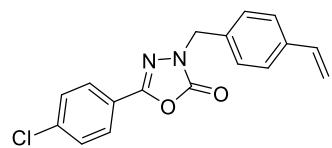


(Scheme 3, 3d);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

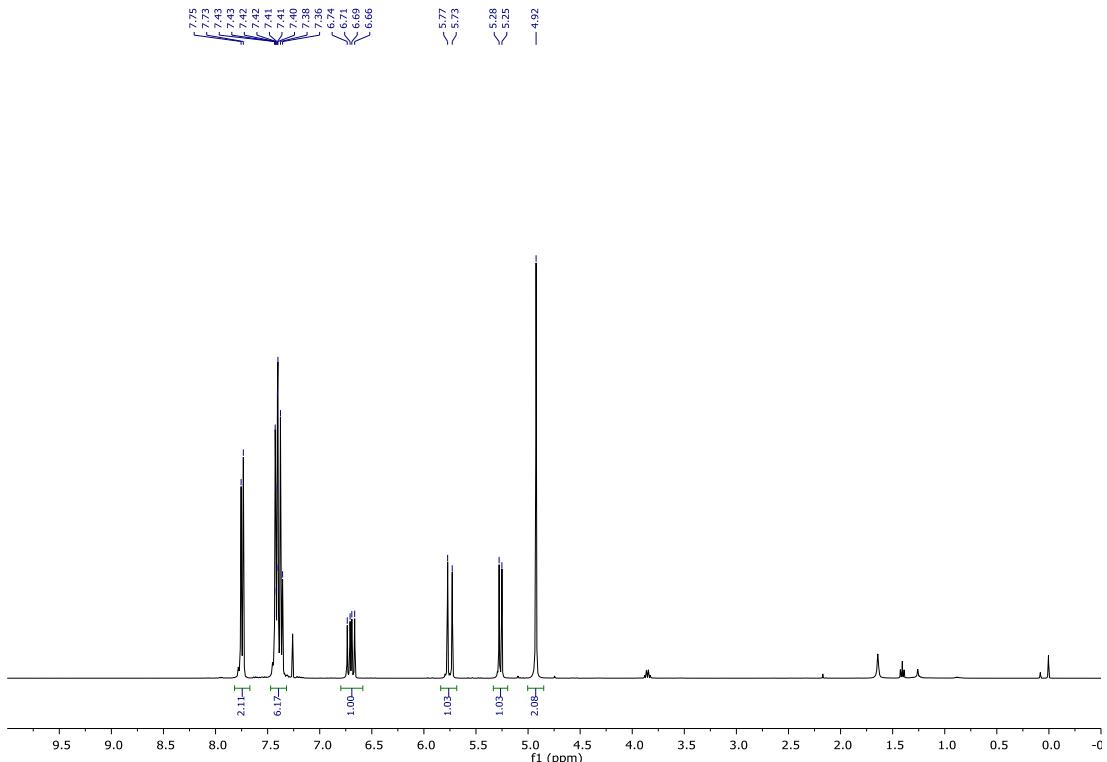


(Scheme 3, 3d);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

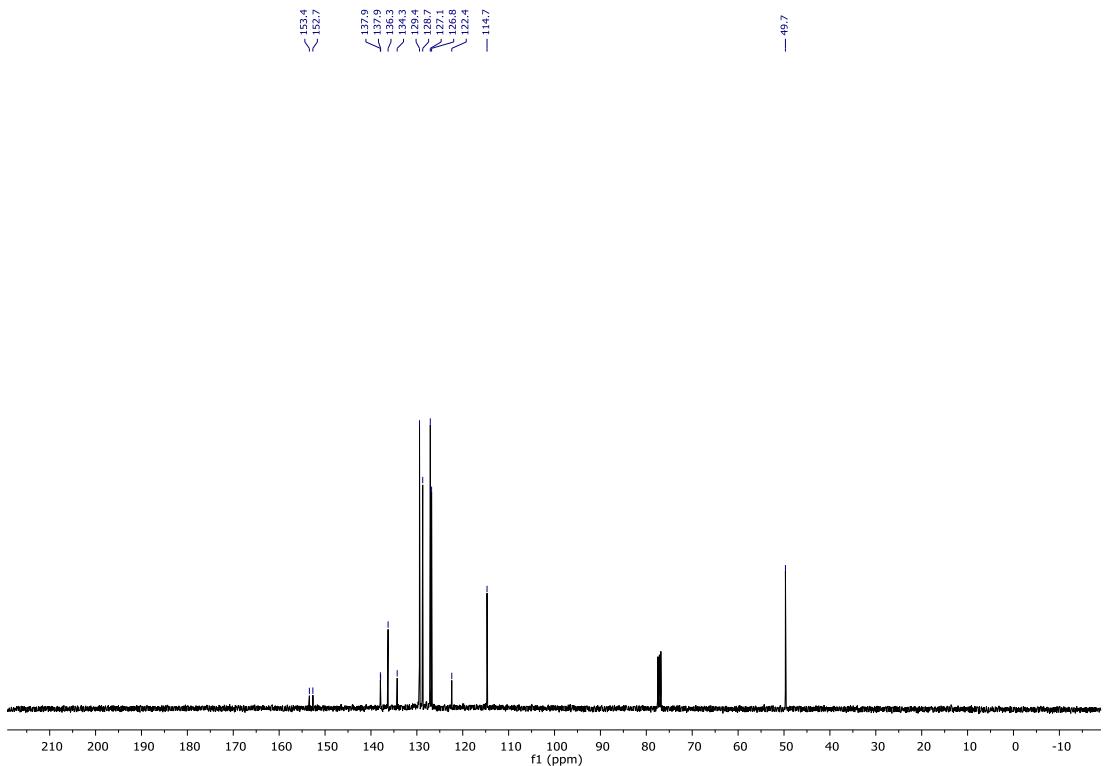


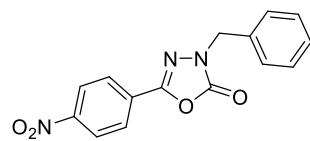


(Scheme 3, **3e**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

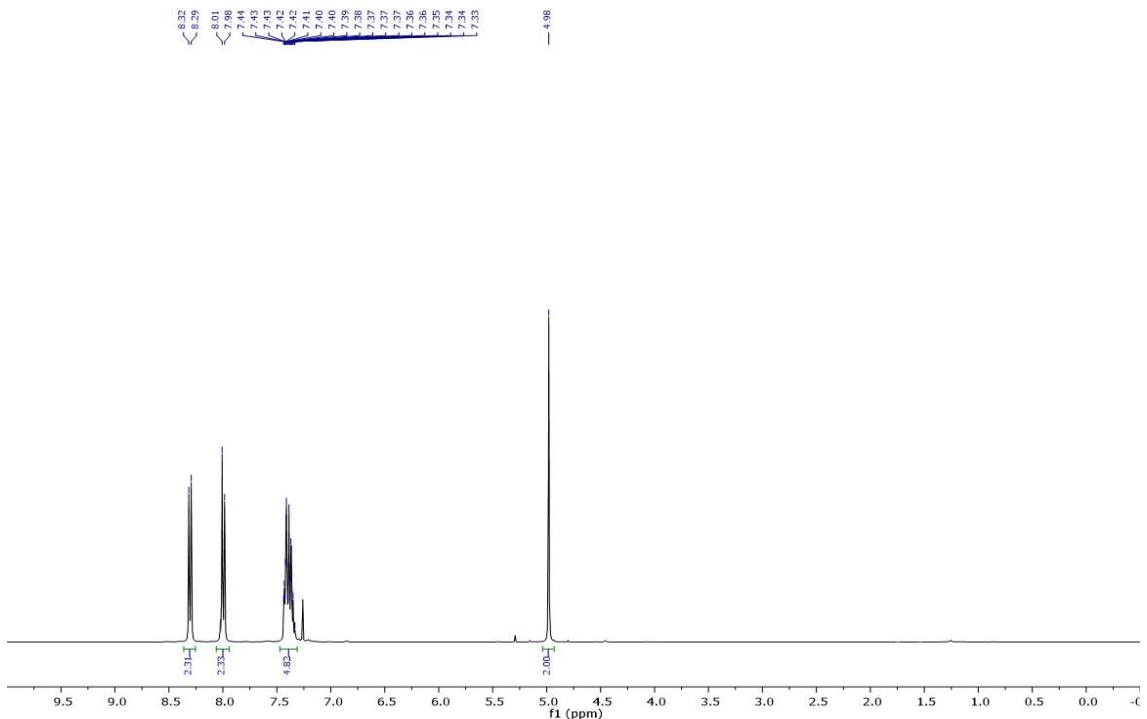


(Scheme 3, **3e**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

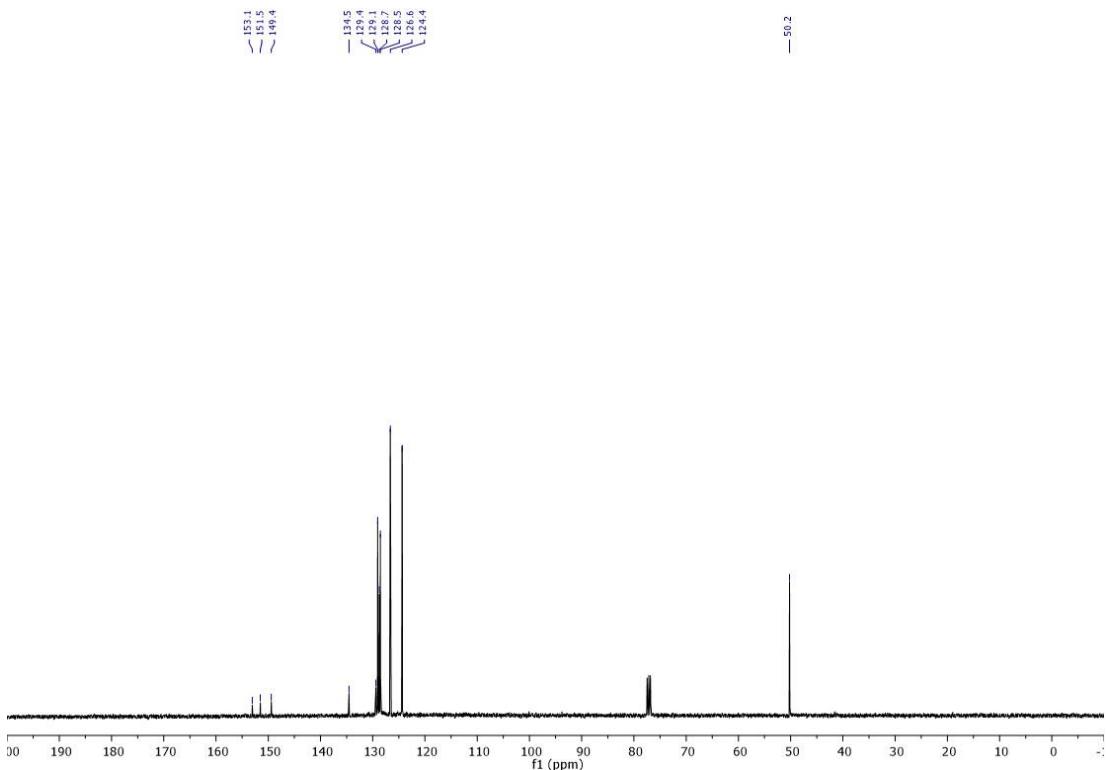


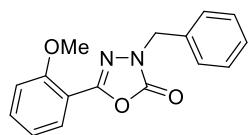


(Scheme 3, **3f**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

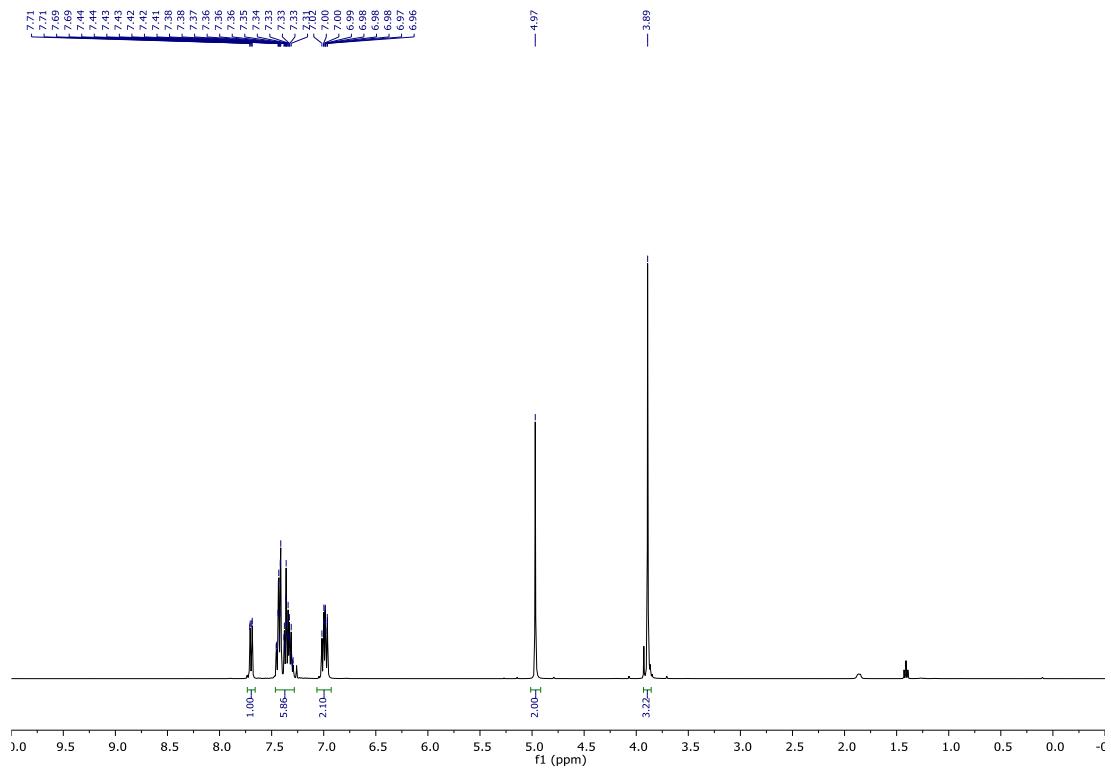


(Scheme 3, **3f**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

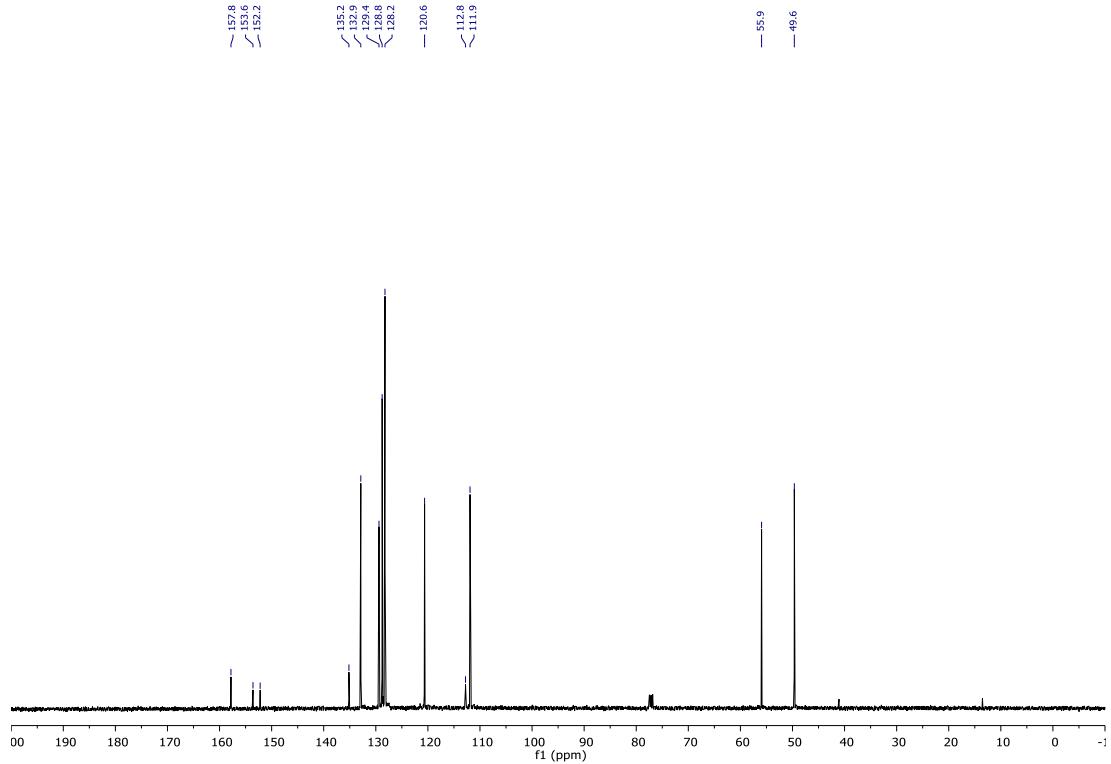


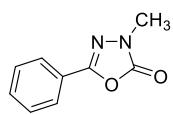


(Scheme 3, 3g);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

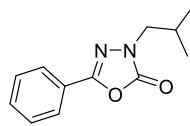
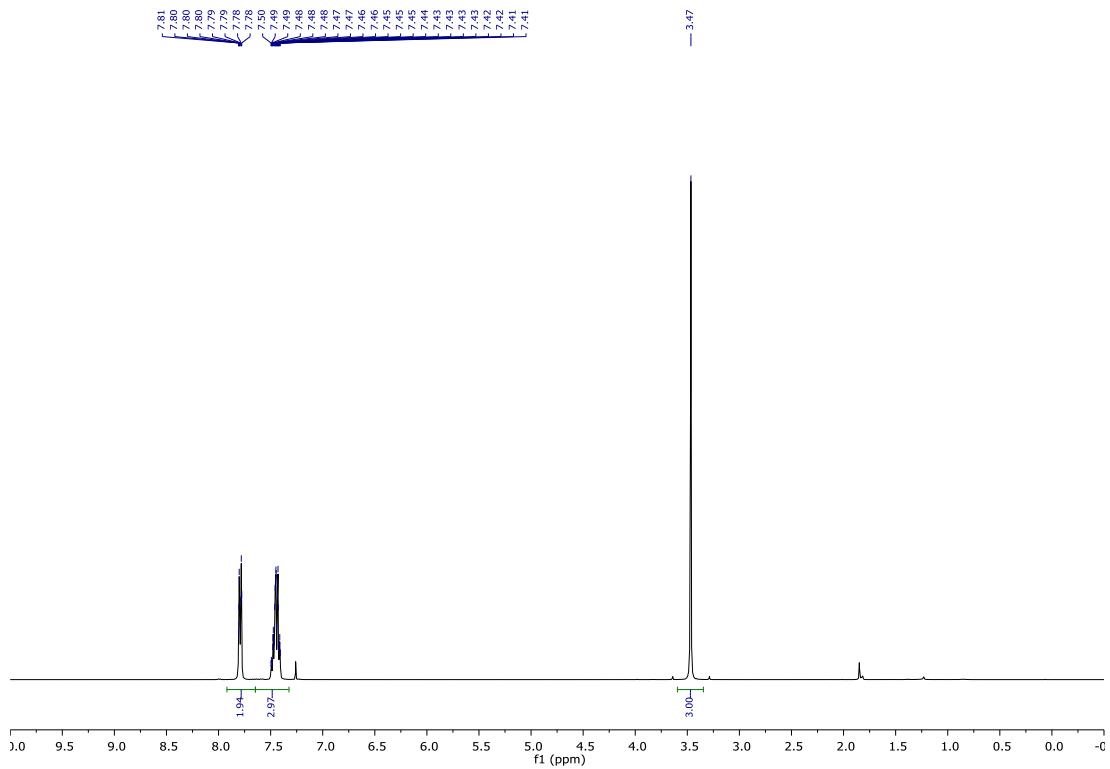


(Scheme 3, 3g);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

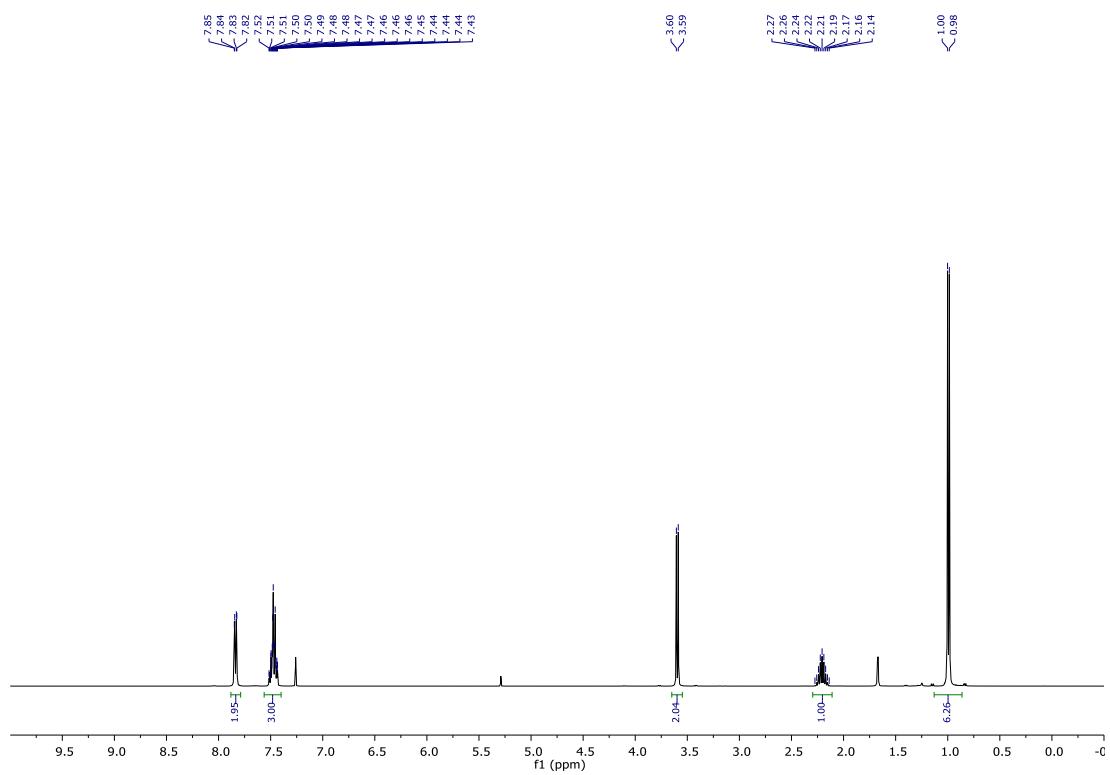


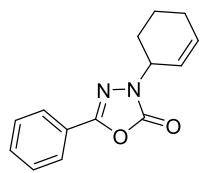


(Scheme 3, **3h**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

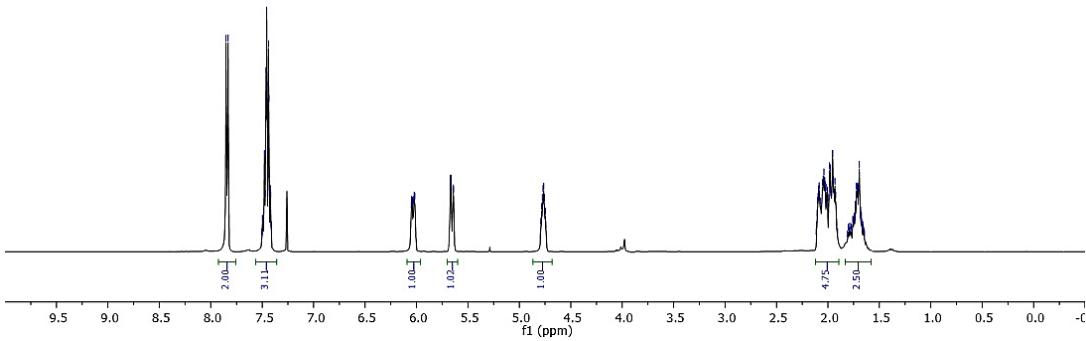


(Scheme, 3i);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

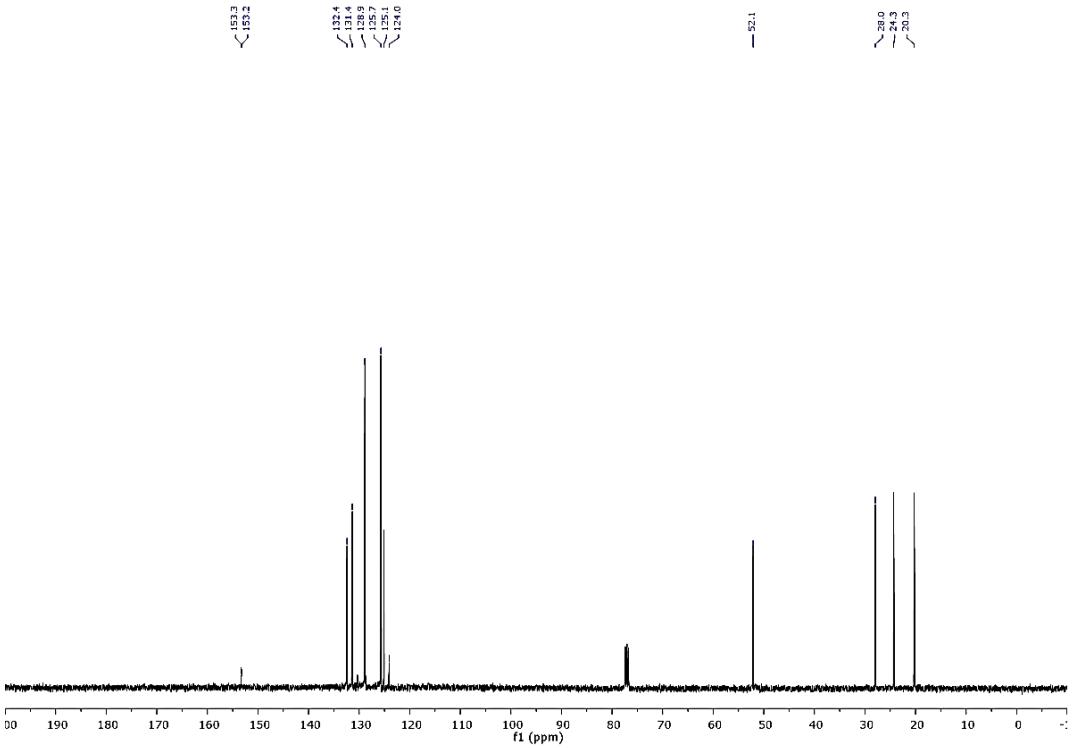


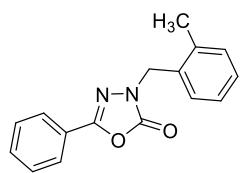


(Scheme 3, 3j);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

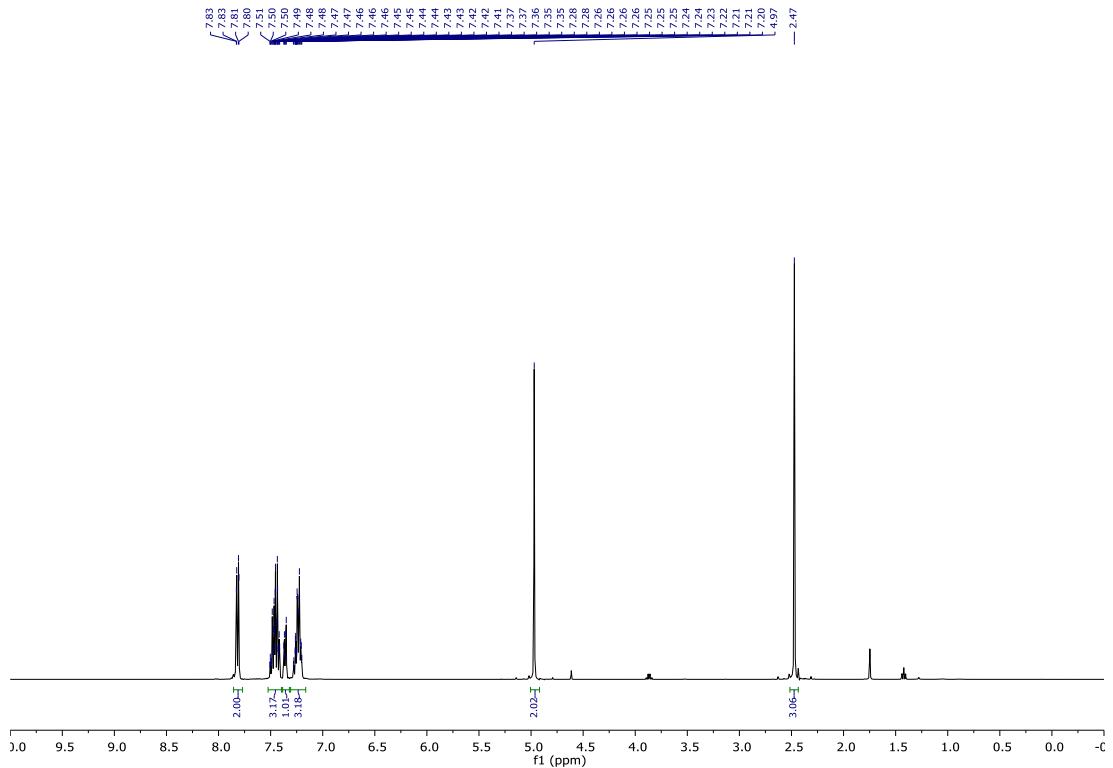


(Scheme 3, **3j**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

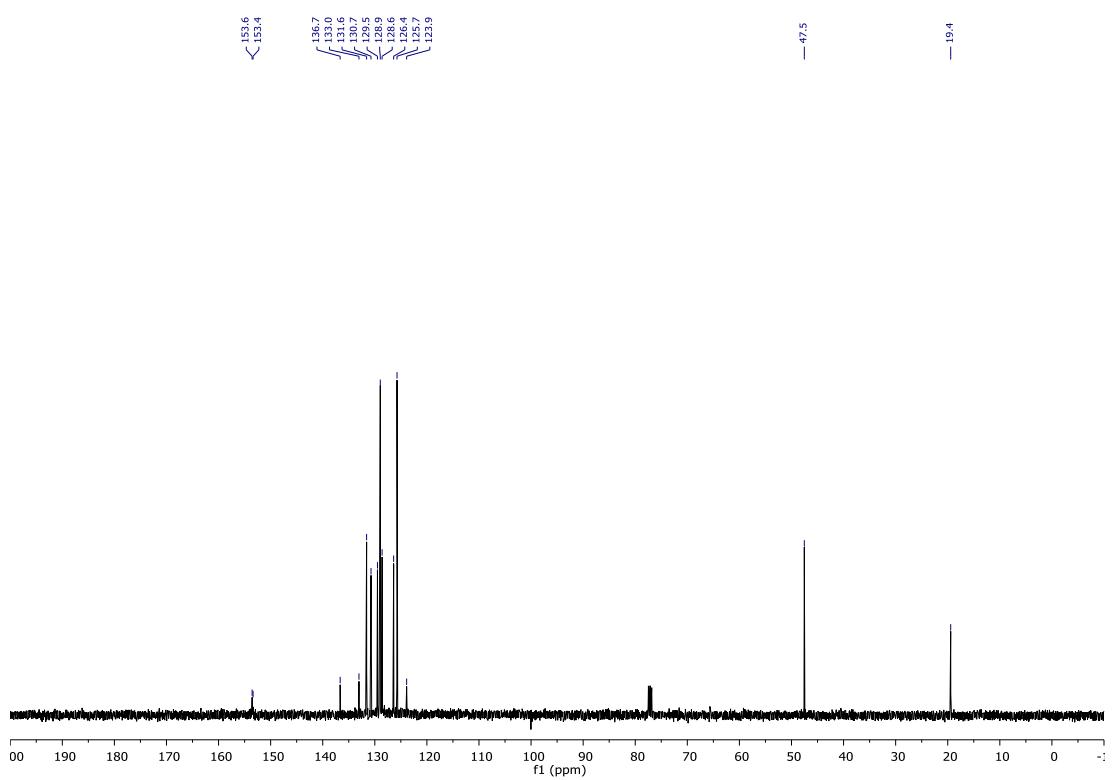


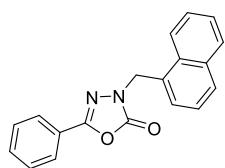


(Scheme 3, **3l**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

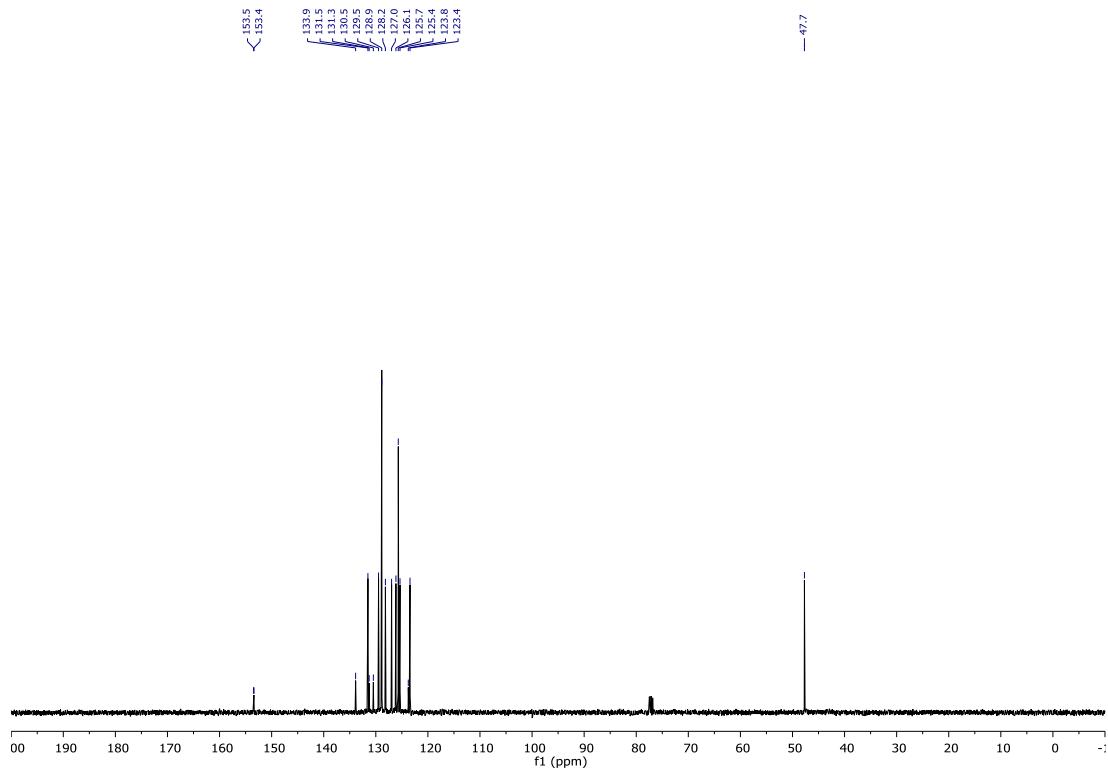
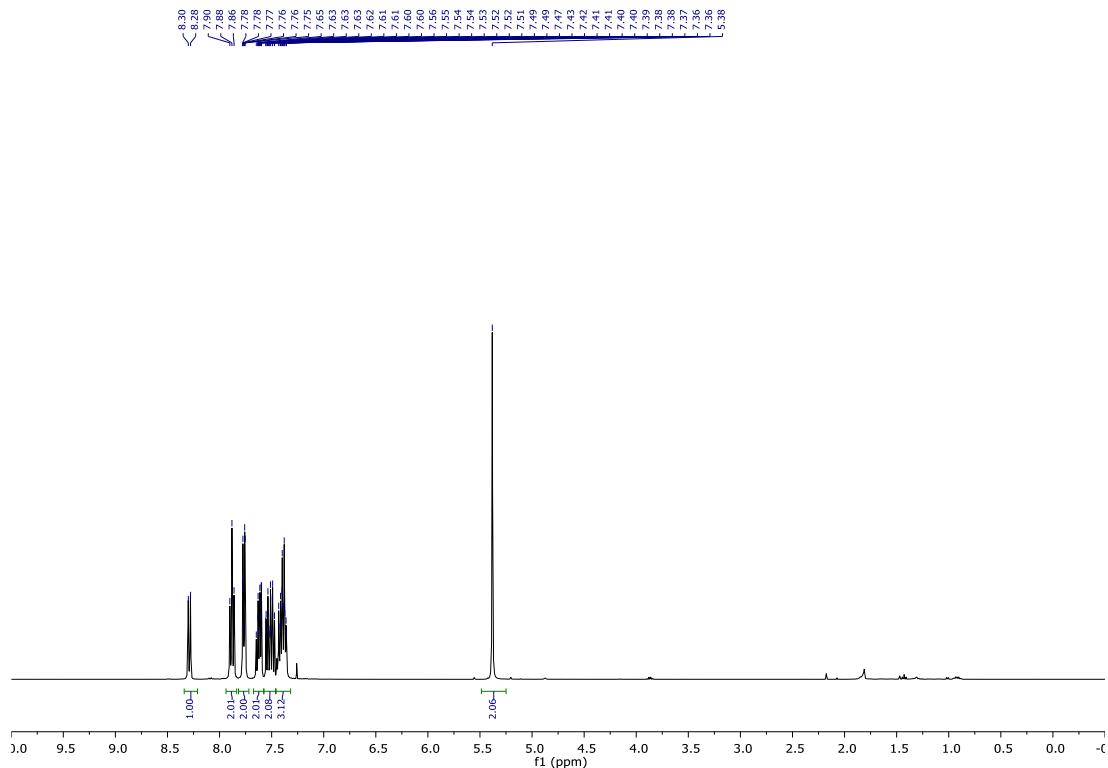


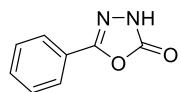
(Scheme 3, **3l**);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )



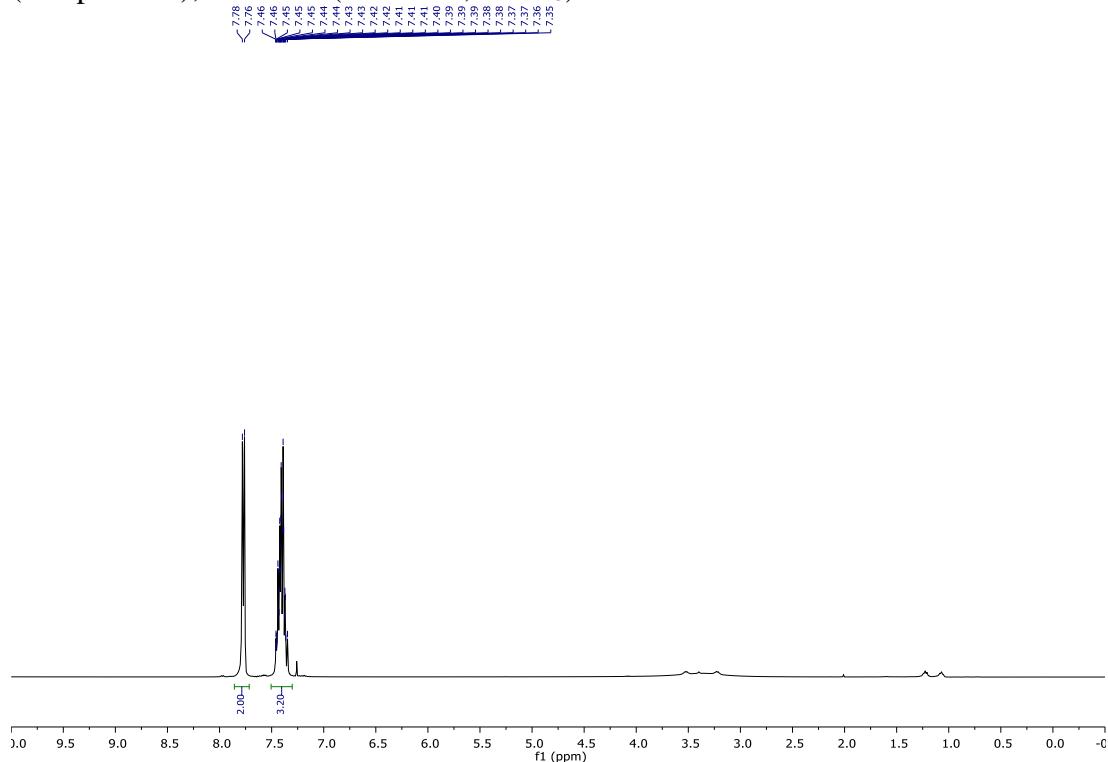


(Scheme 3, **3m**);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

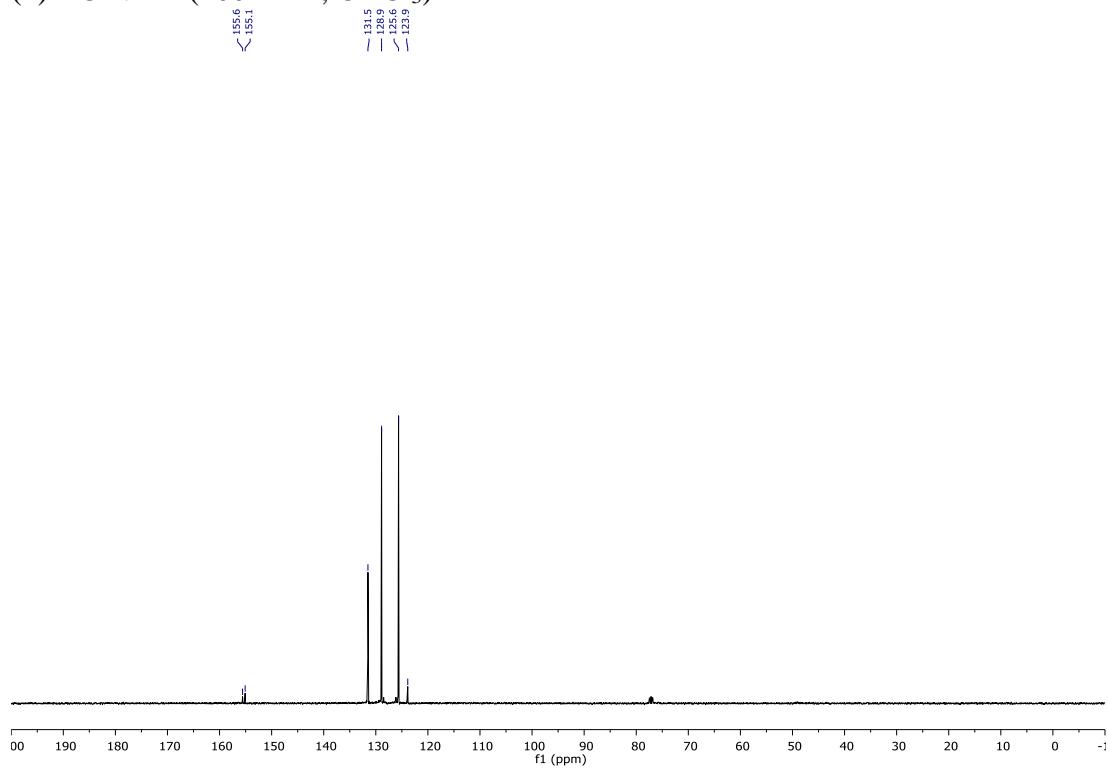




(compound 4);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

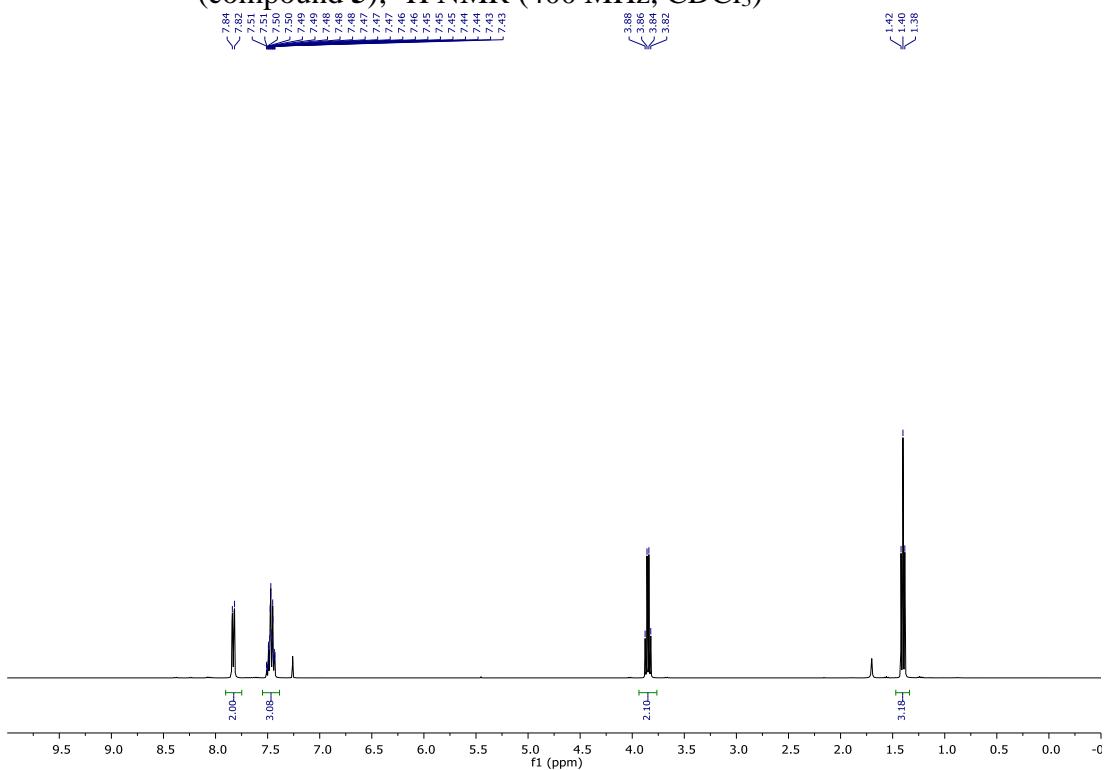


(4)  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

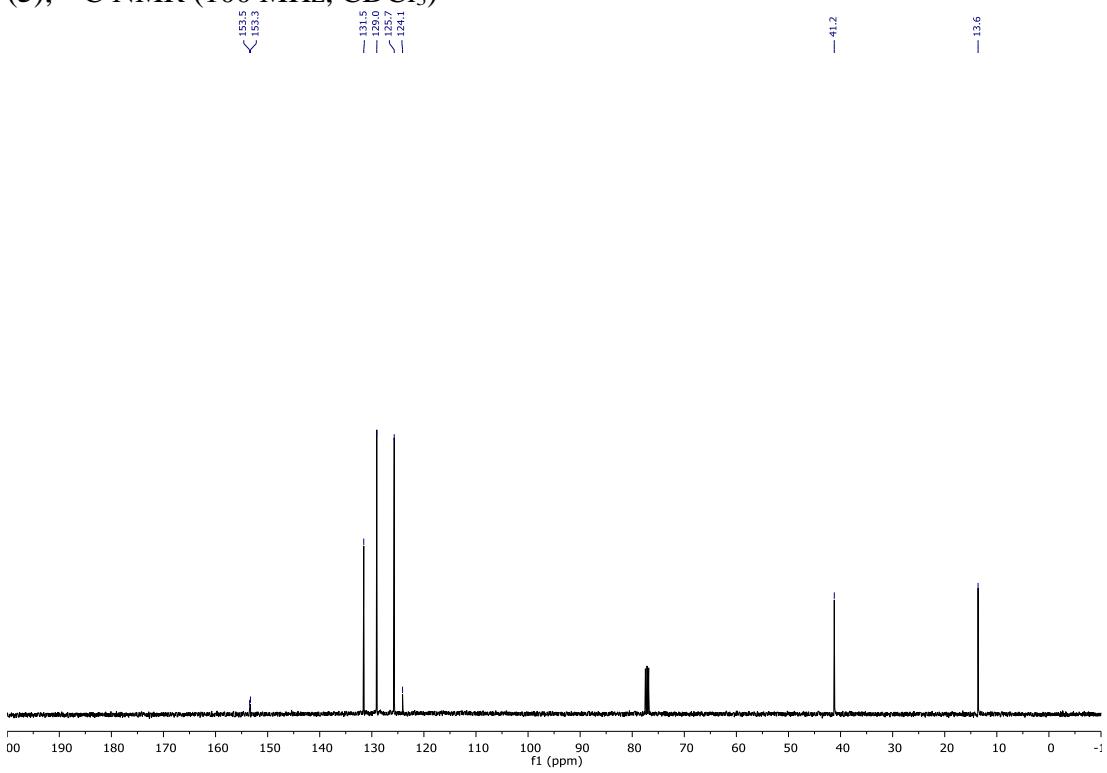


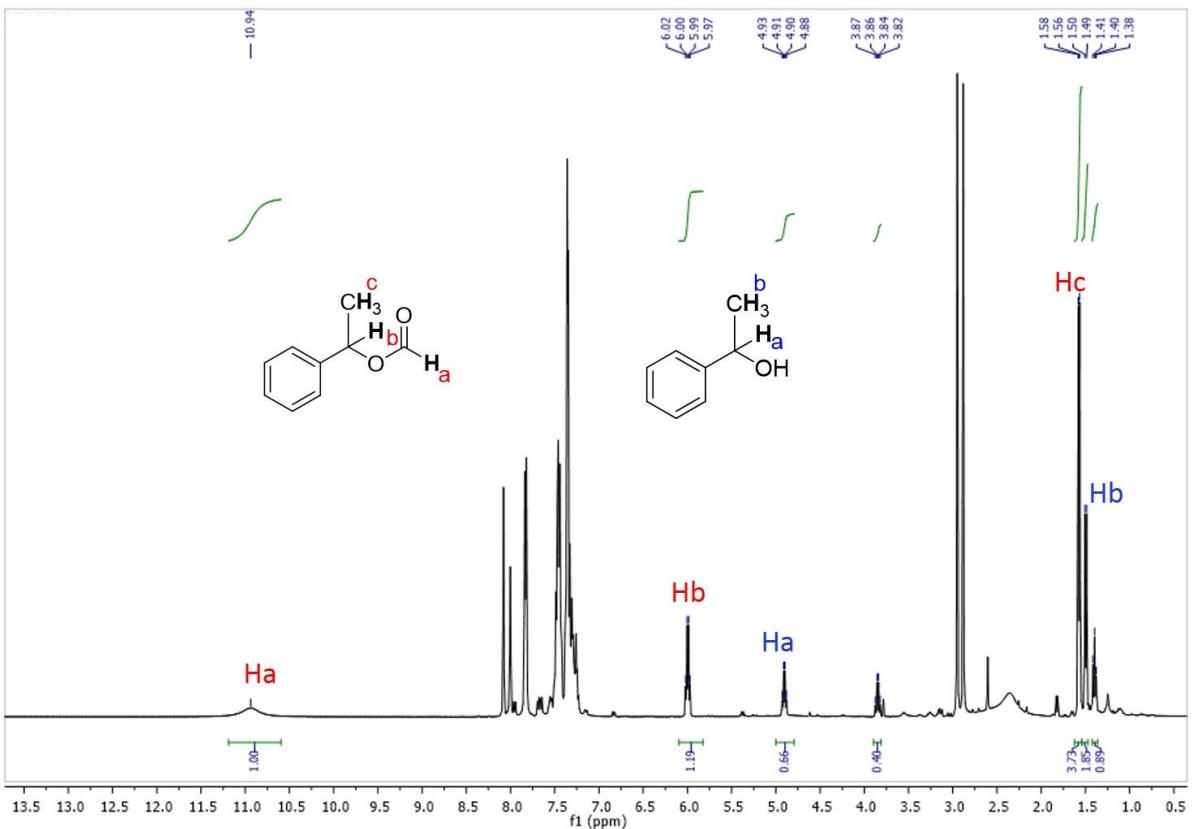
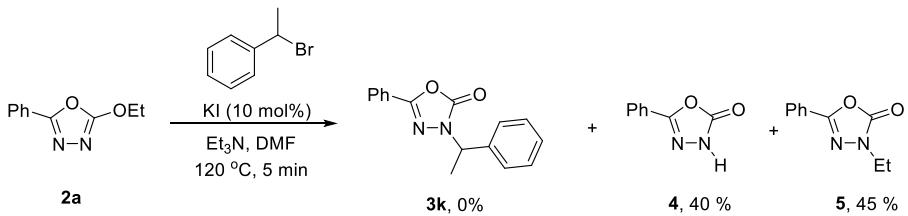


(compound 5);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



(5);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )





**Figure S1**  $^1\text{H}$  NMR spectrum of crude products from the reaction of **2a** with (1-bromoethyl)benzene after extraction with 1N HCl and  $\text{CH}_2\text{Cl}_2$ .