

π -Extension of a 4-Ethoxy-1,3-thiazole via Aryl Alkyne Cross Coupling: Synthesis and Exploration of Electronic Structure

- Electronic Supplementary Information -

Stefanie H. Habenicht^a, Stefan Schramm^a, Mingming Zhu^a, Robert R. A. Freund^a, Teresa Langenstück^b, Rainer Strathausen^{a,b}, Dieter Weiß^a, Christoph Biskup^b and Rainer Beckert^{*a}

¹Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich Schiller University, Humboldtstr. 10, 07743 Jena, Germany

²Biomolecular Photonics Group, Jena University Hospital, Friedrich Schiller University, Nonnenplan 2-4, 07743 Jena, Germany

Email:

Rainer Beckert* - Rainer.Beckert@uni-jena.de

*Corresponding author

Table of Contents

1. Table S1	page 3
2. Lambert-Beer-plots	page 4
3. ^1H NMR spectra	page 8
4. ^{13}C NMR spectra	page 13

1. Table S1

compound	angle [°]	compound	angle [°]
3a	17.865	6a	20.193
3b	17.195	6b	22.720
3c	15.613	6c	21.916
3d	13.467	-	-

Table S1: calculated torsion angles between thiazole cores and their substituents in 5-position.

2. Lambert-Beer plots

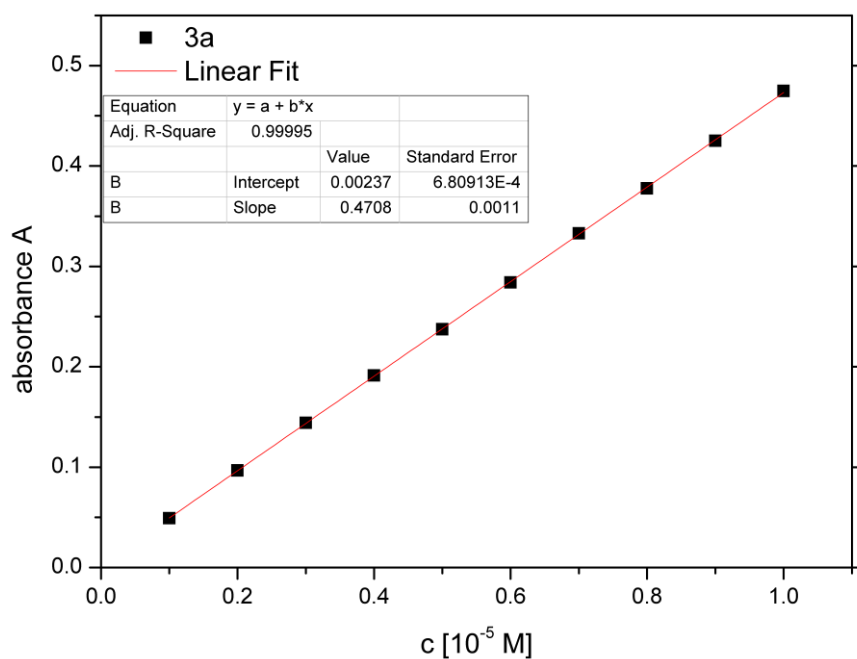


Figure S1: Lambert-Beer-plot for **3a**, 10⁻⁶-10⁻⁵ M in THF.

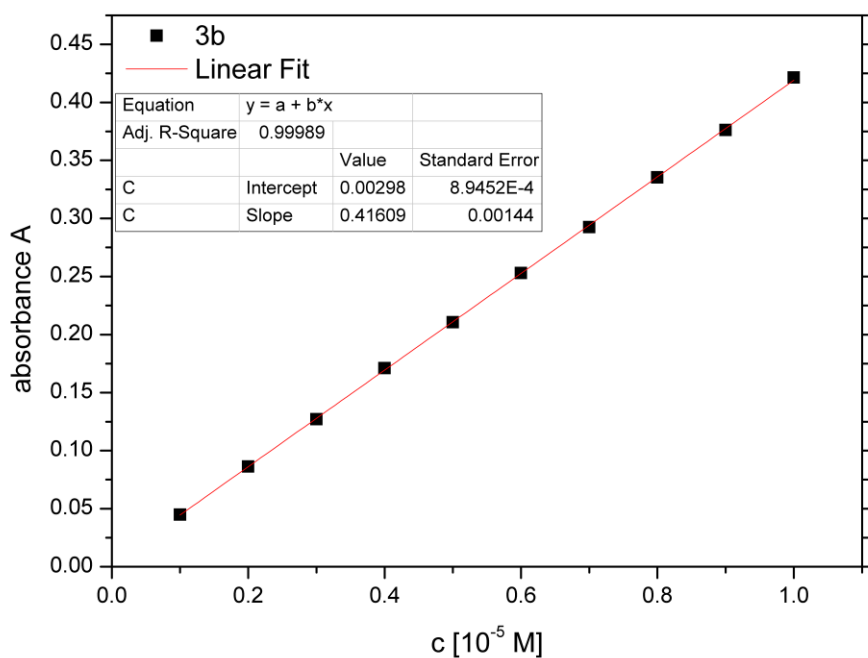


Figure S2: Lambert-Beer-plot for **3b**, 10⁻⁶-10⁻⁵ M in THF.

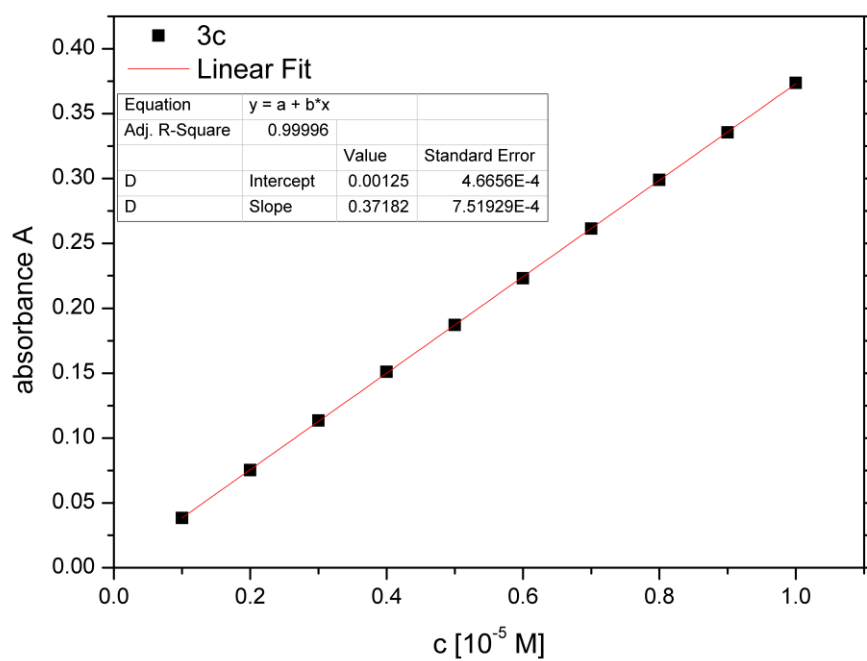


Figure S3: Lambert-Beer-plot for **3c**, 10^{-6} - 10^{-5} M in THF.

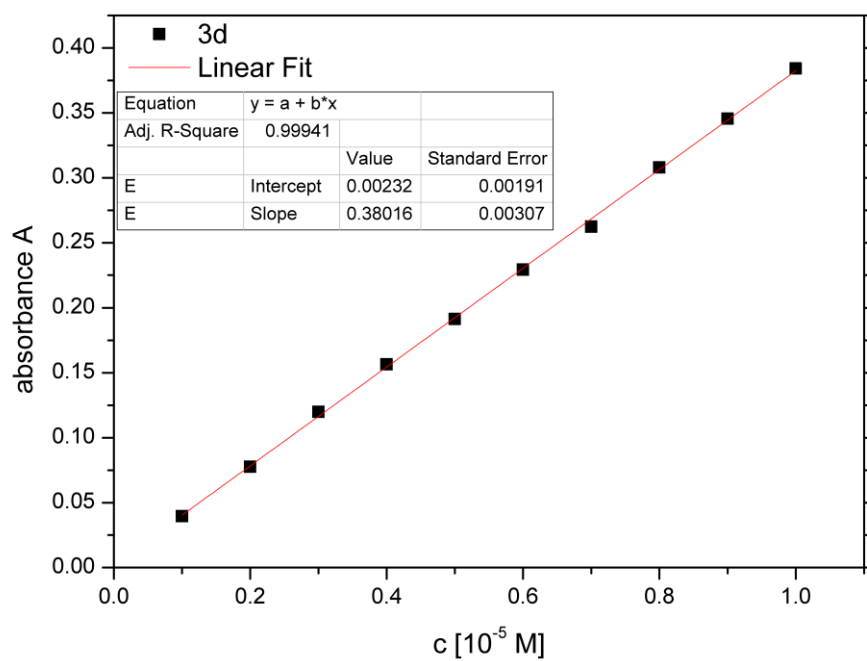


Figure S4: Lambert-Beer-plot for **3d**, 10^{-6} - 10^{-5} M in THF.

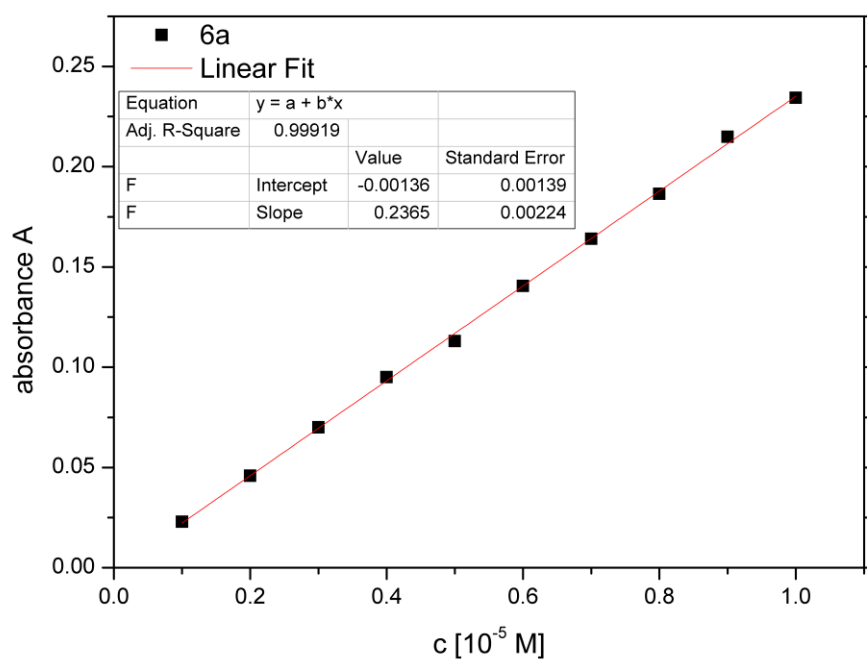


Figure S5: Lambert-Beer-plot for **6a**, 10^{-6} - 10^{-5} M in THF.

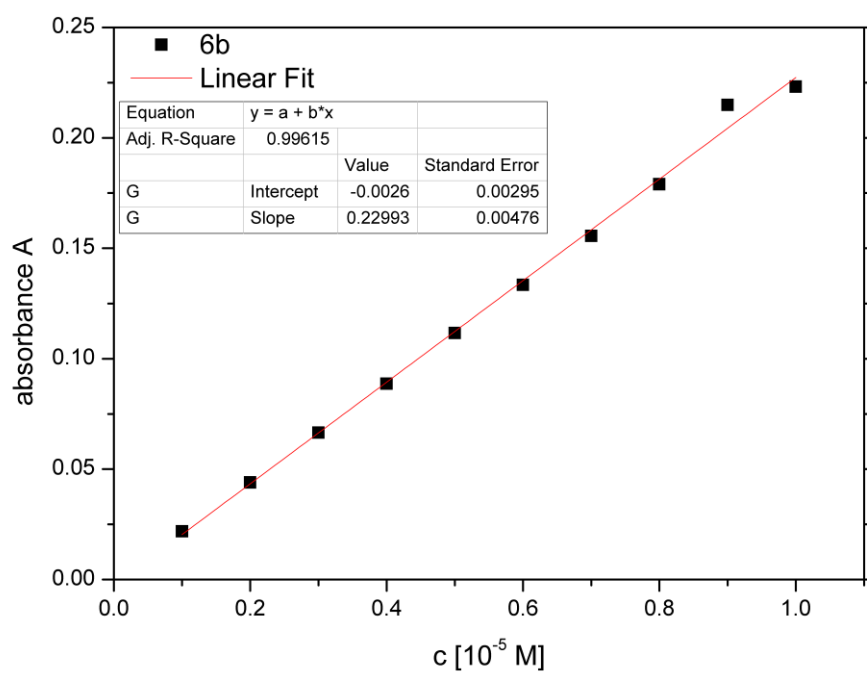


Figure S6: Lambert-Beer-plot for **6b**, 10^{-6} - 10^{-5} M in THF.

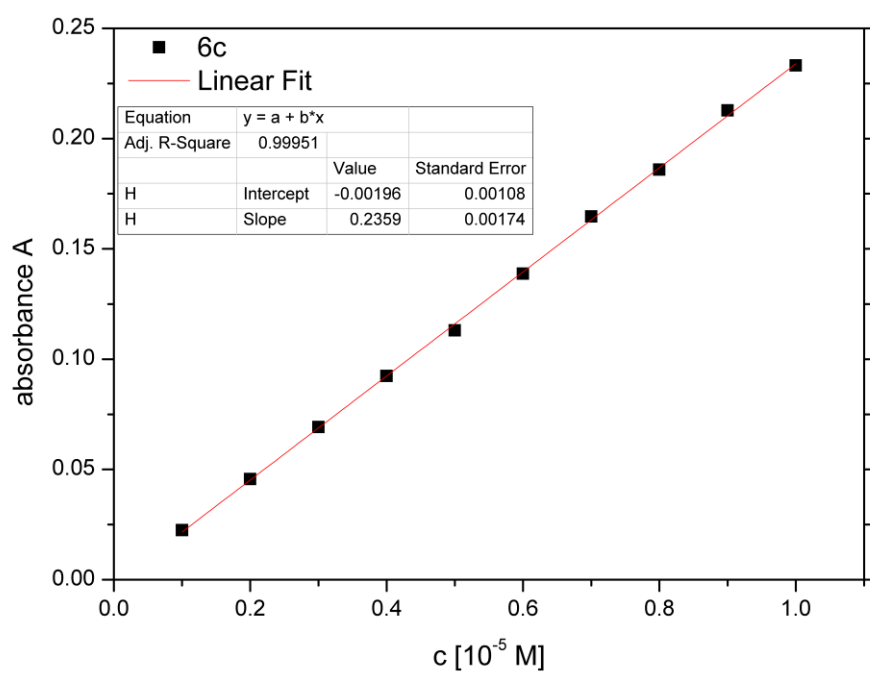


Figure S7: Lambert-Beer-plot for **6c**, 10^{-6} - 10^{-5} M in THF.

3. ^1H NMR spectra

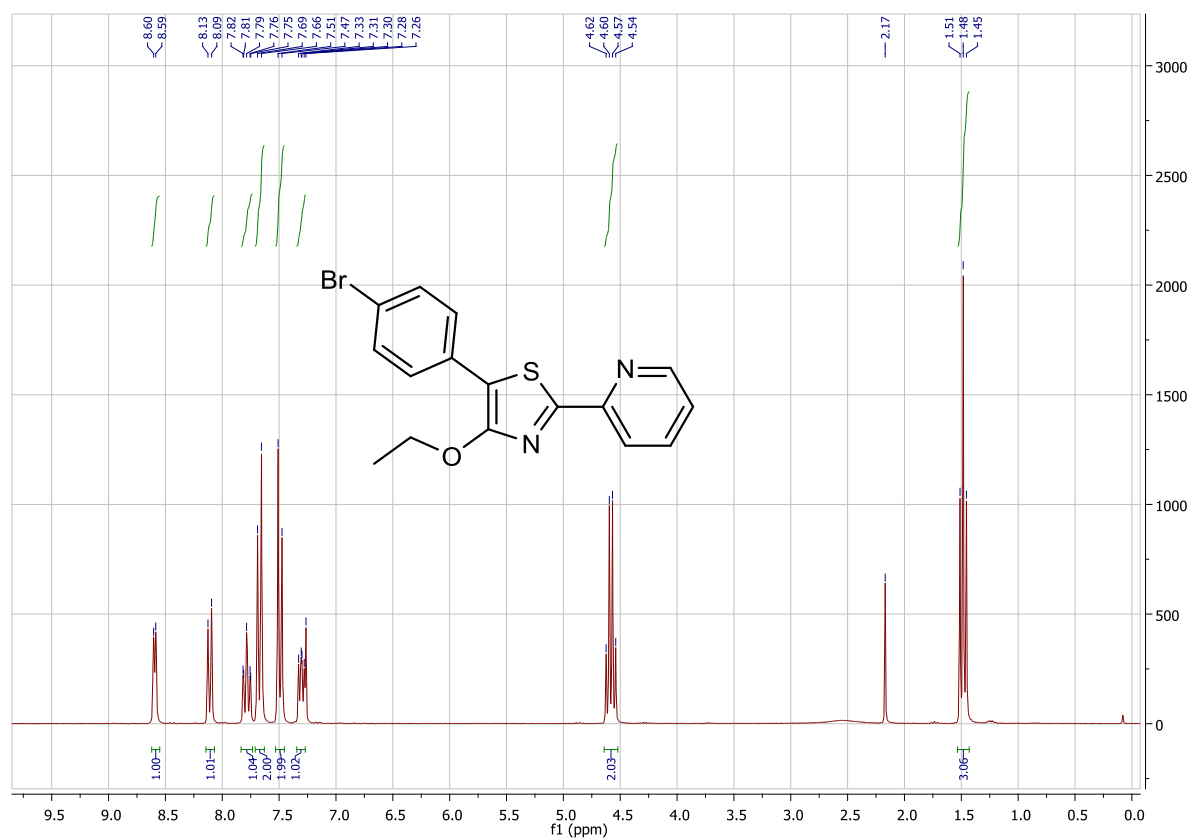


Figure S8: ^1H NMR spectrum of 2.

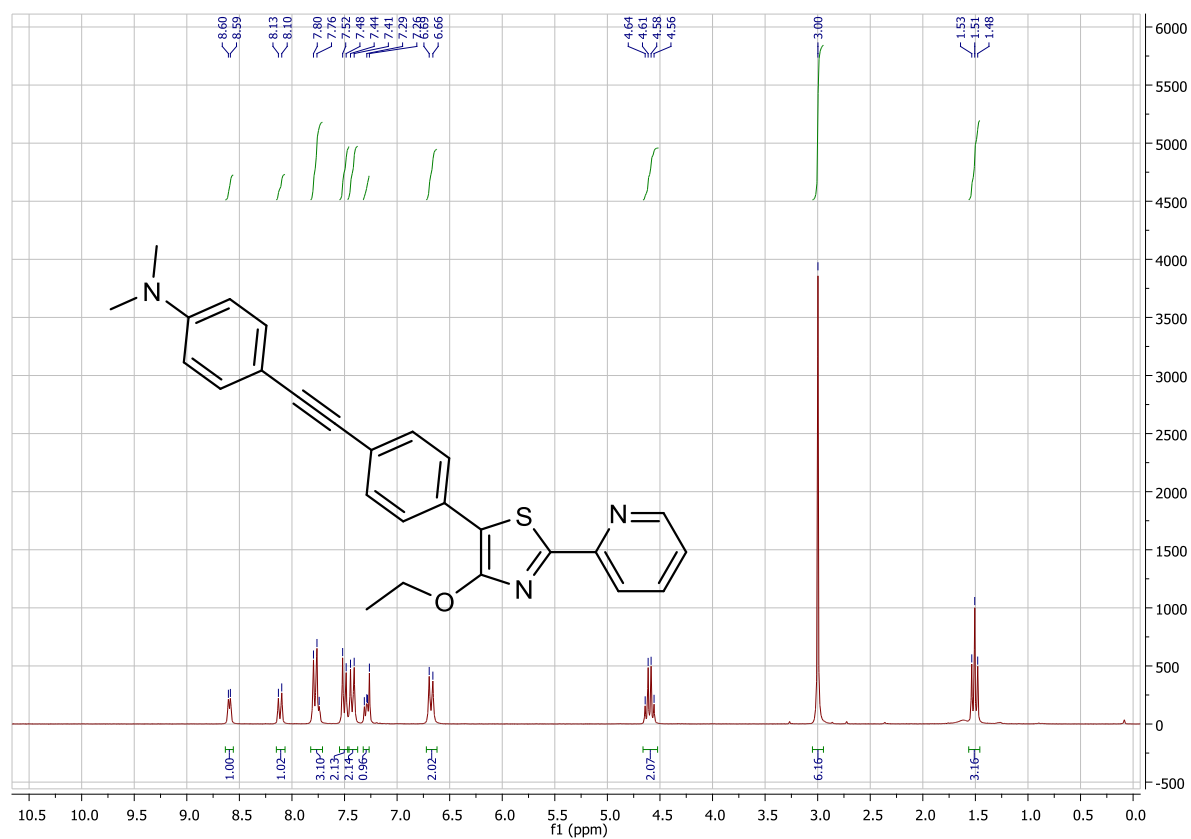


Figure S9: ^1H NMR spectrum of 3a.

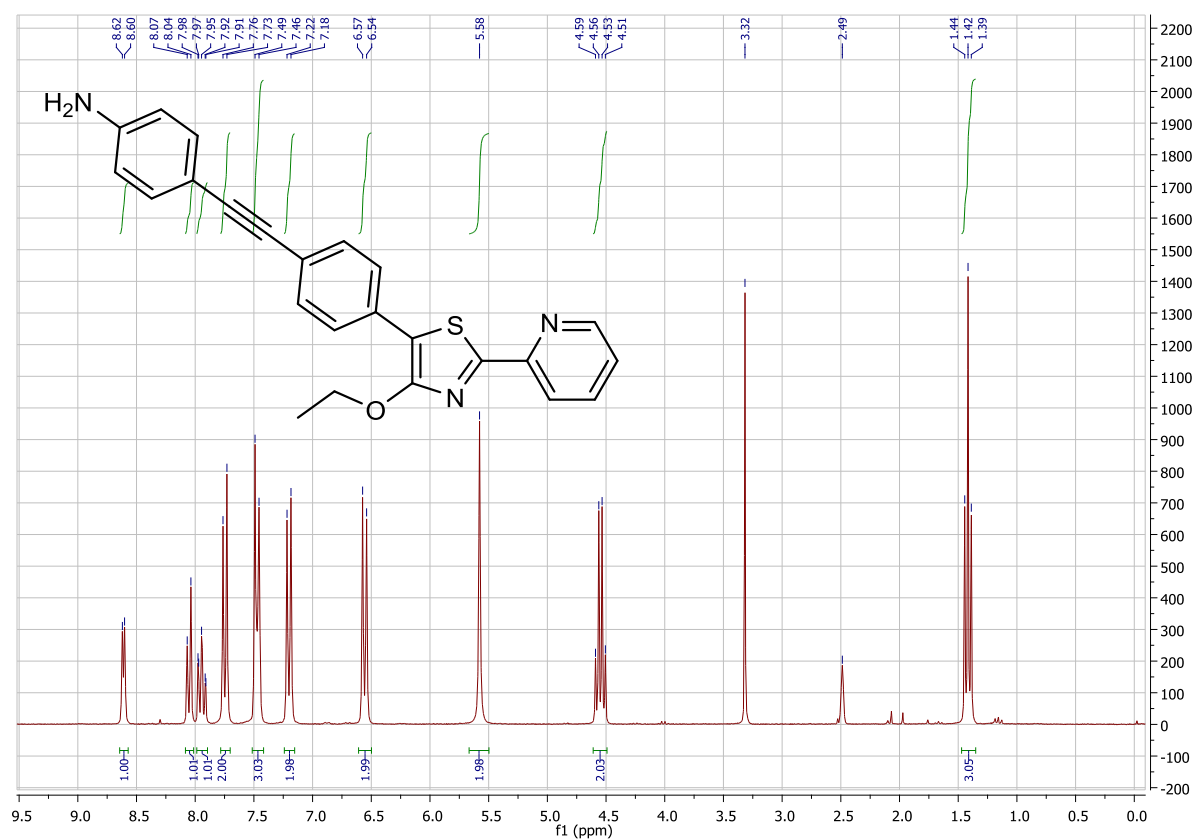


Figure S10: ^1H NMR spectrum of 3b.

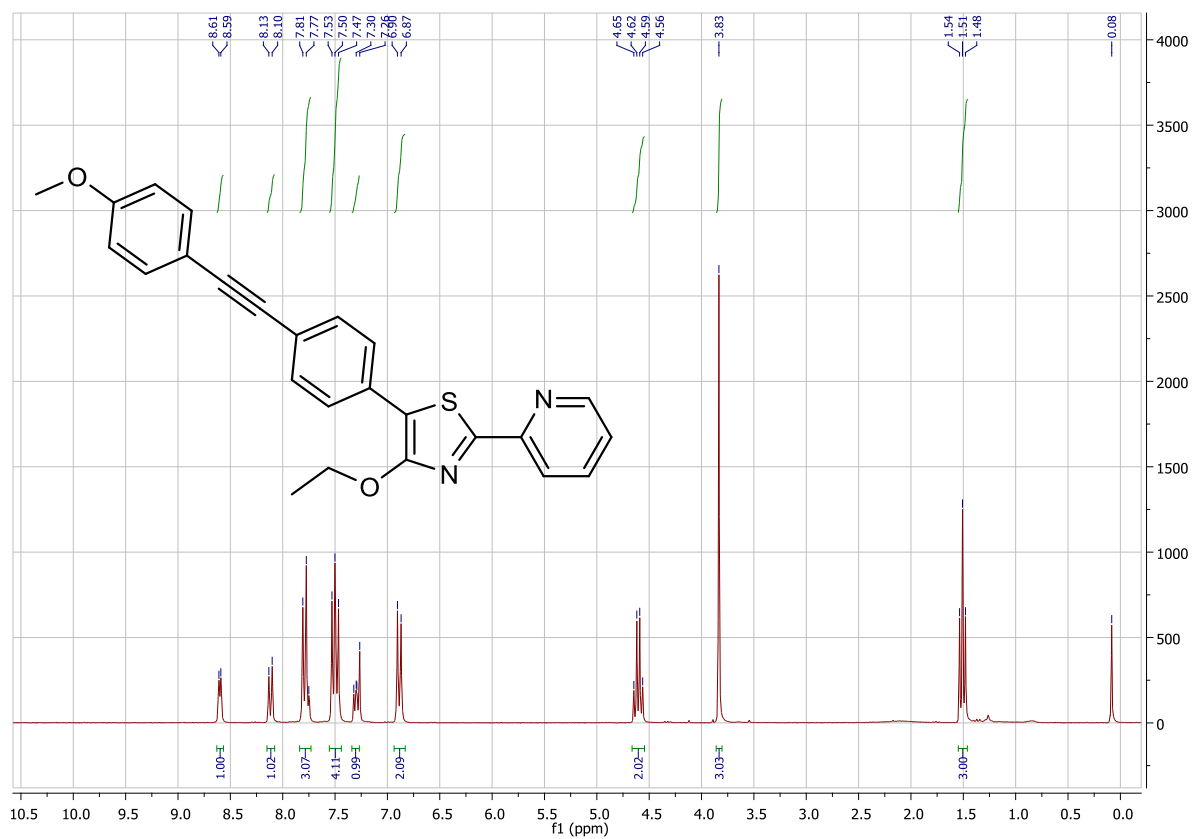


Figure S11: ^1H NMR spectrum of 3c.

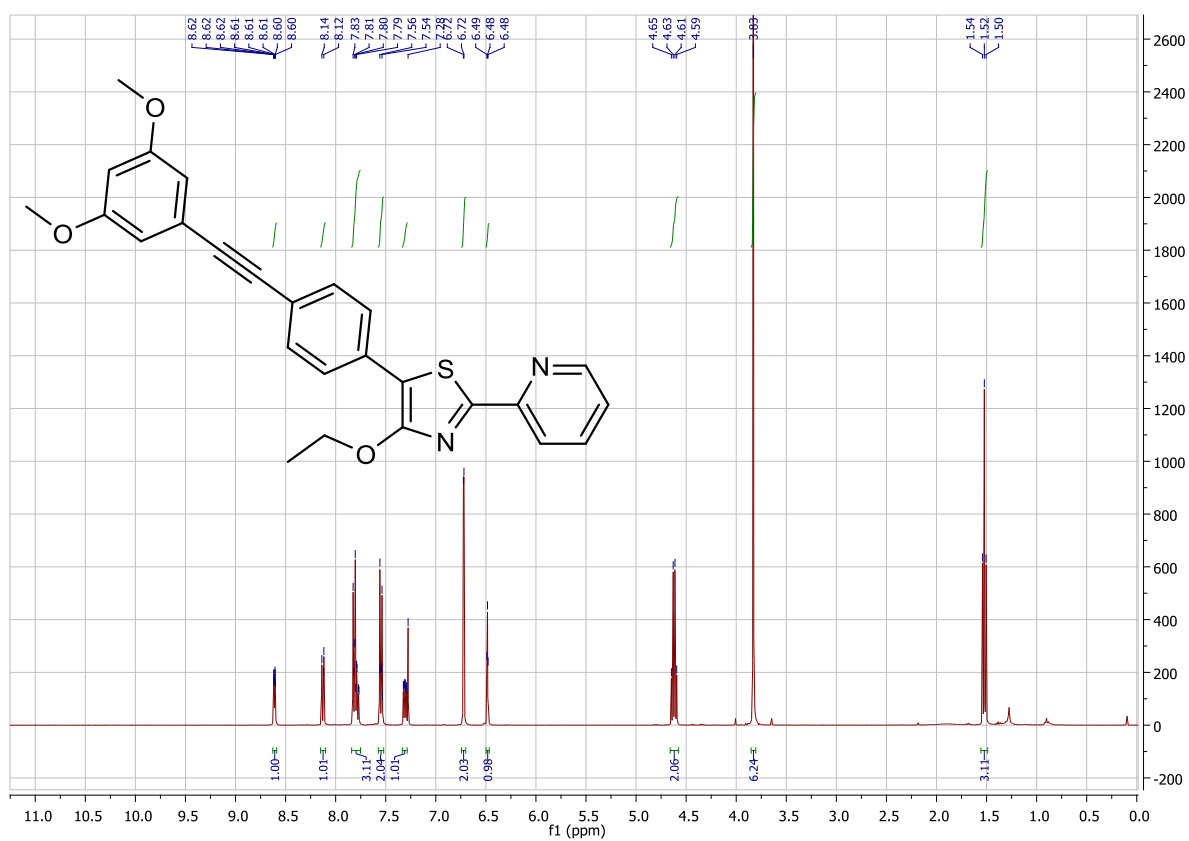


Figure S12: ¹H NMR spectrum of 3d.

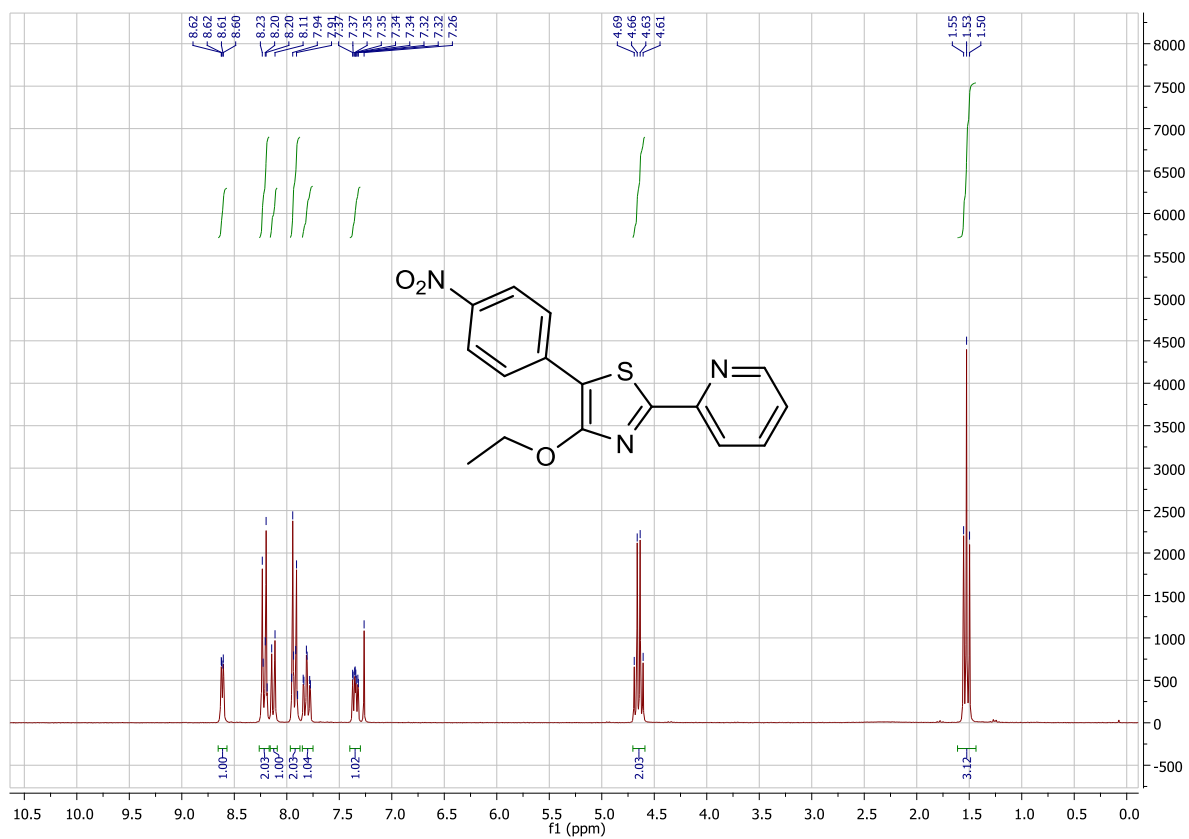


Figure S13: ¹H NMR spectrum of 5.

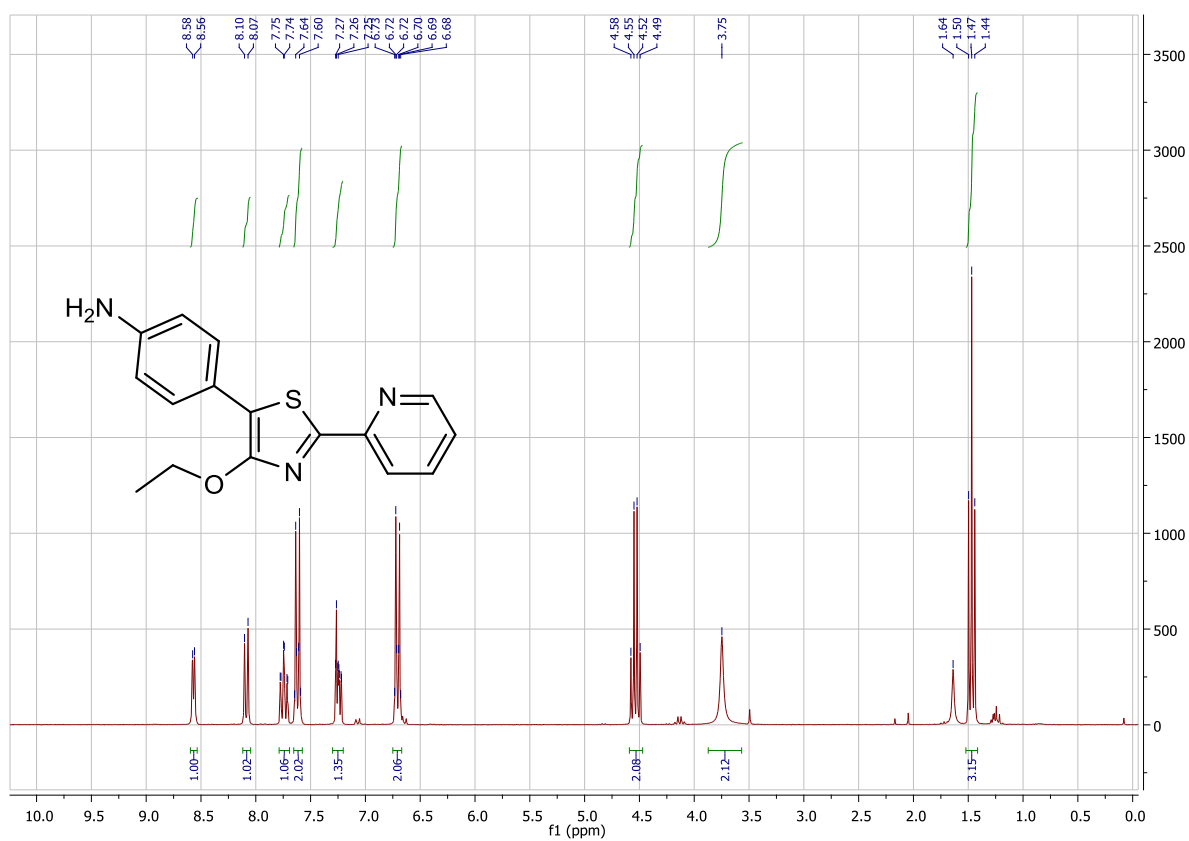


Figure S14: ¹H NMR spectrum of 6b.

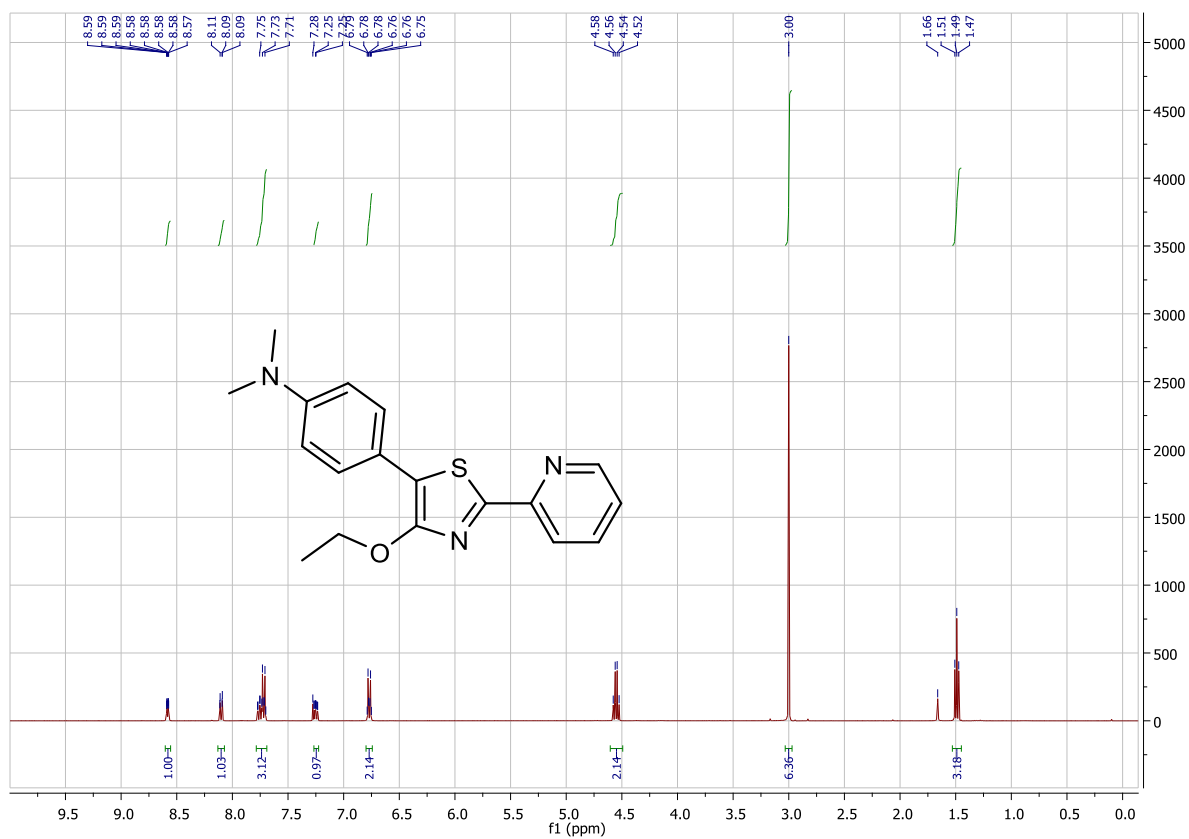


Figure S15: ¹H NMR spectrum of 6a.

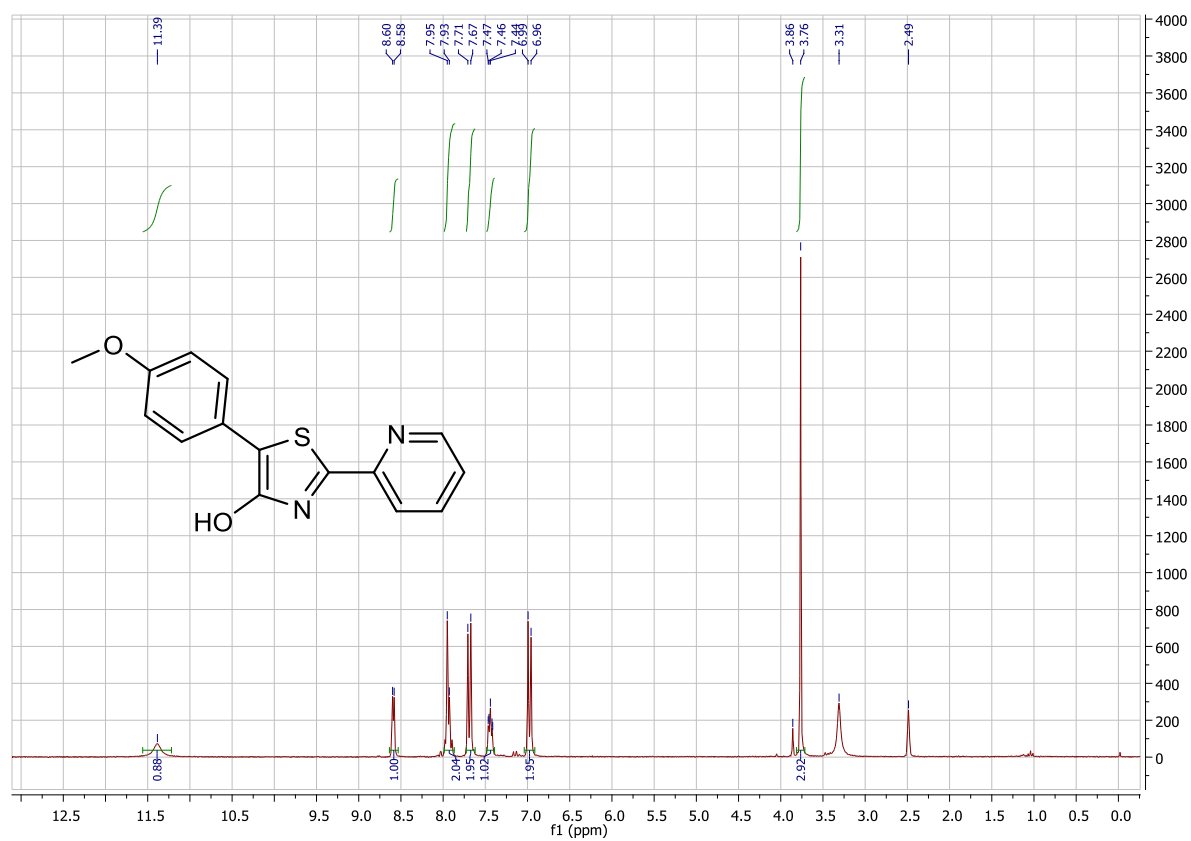


Figure S16: ¹H NMR spectrum of 9.

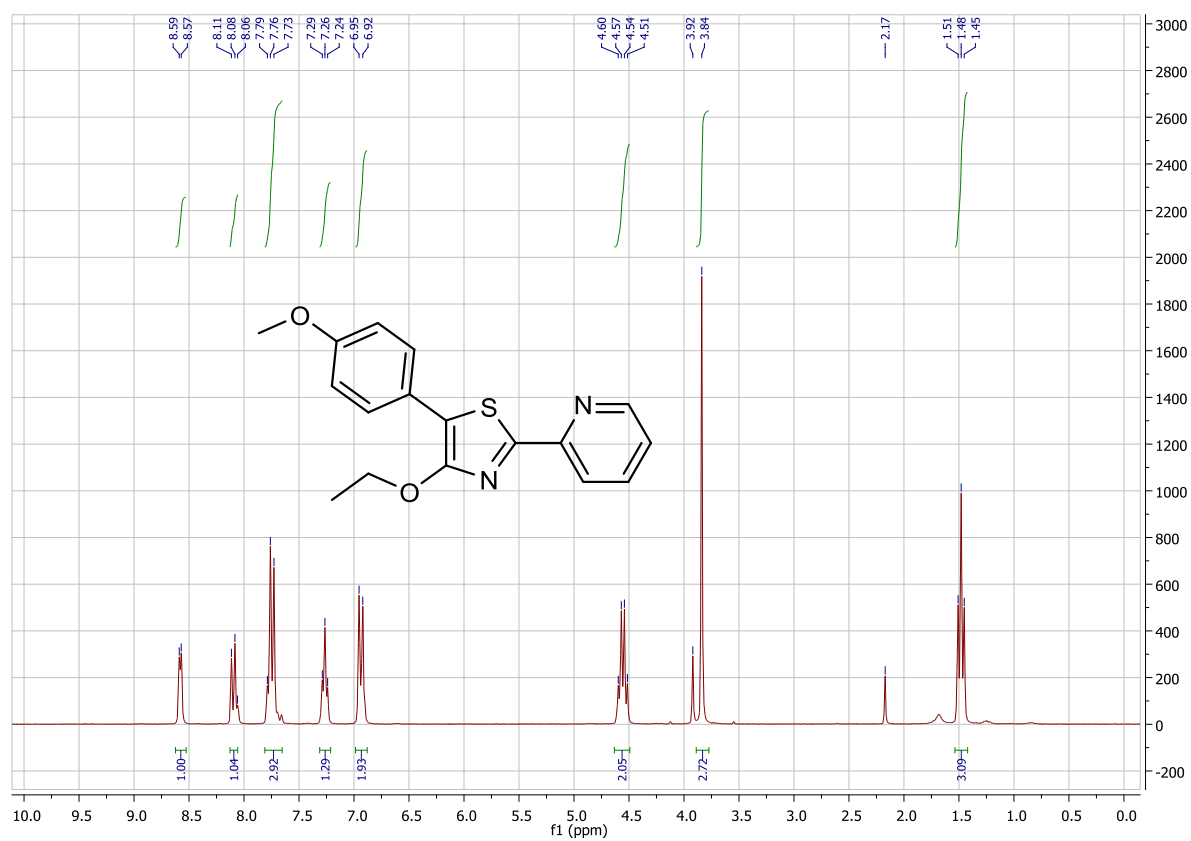


Figure S17: ¹H NMR spectrum of 6c.

4. ^{13}C NMR spectra

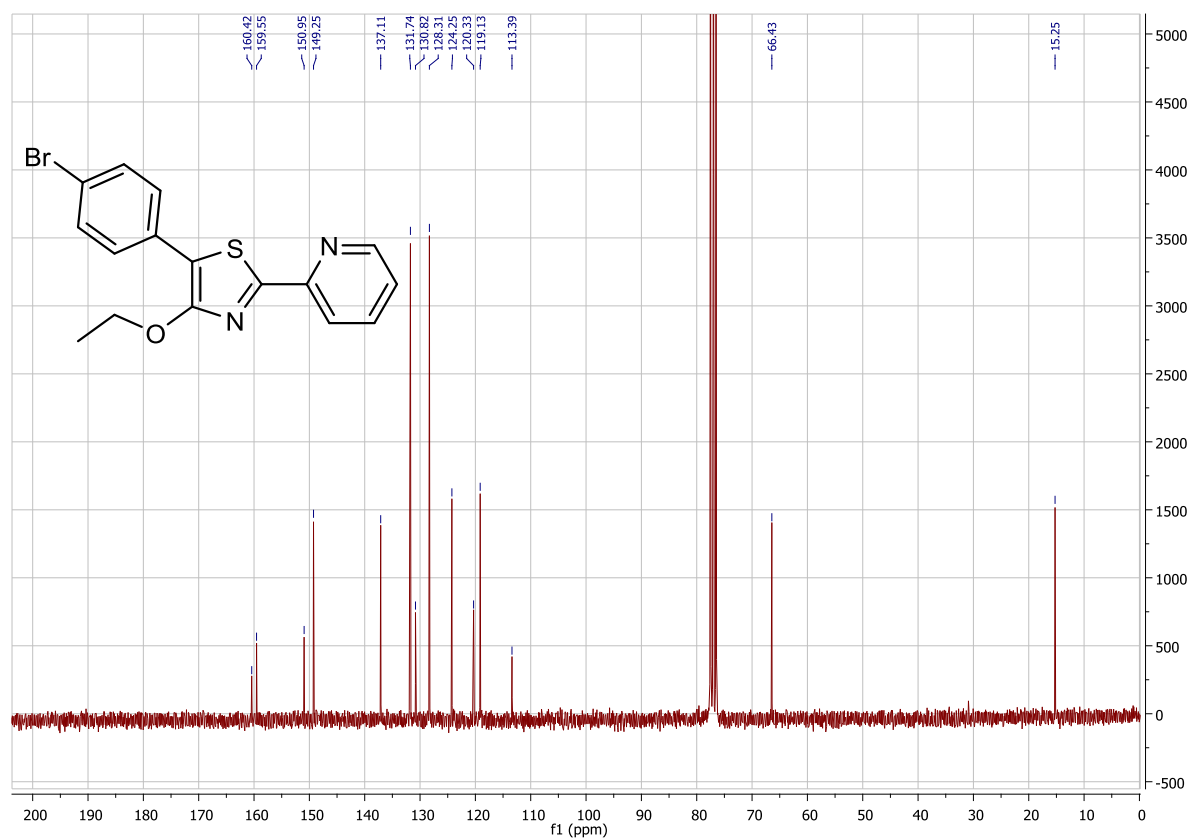


Figure S18: ^{13}C NMR spectrum of 2.

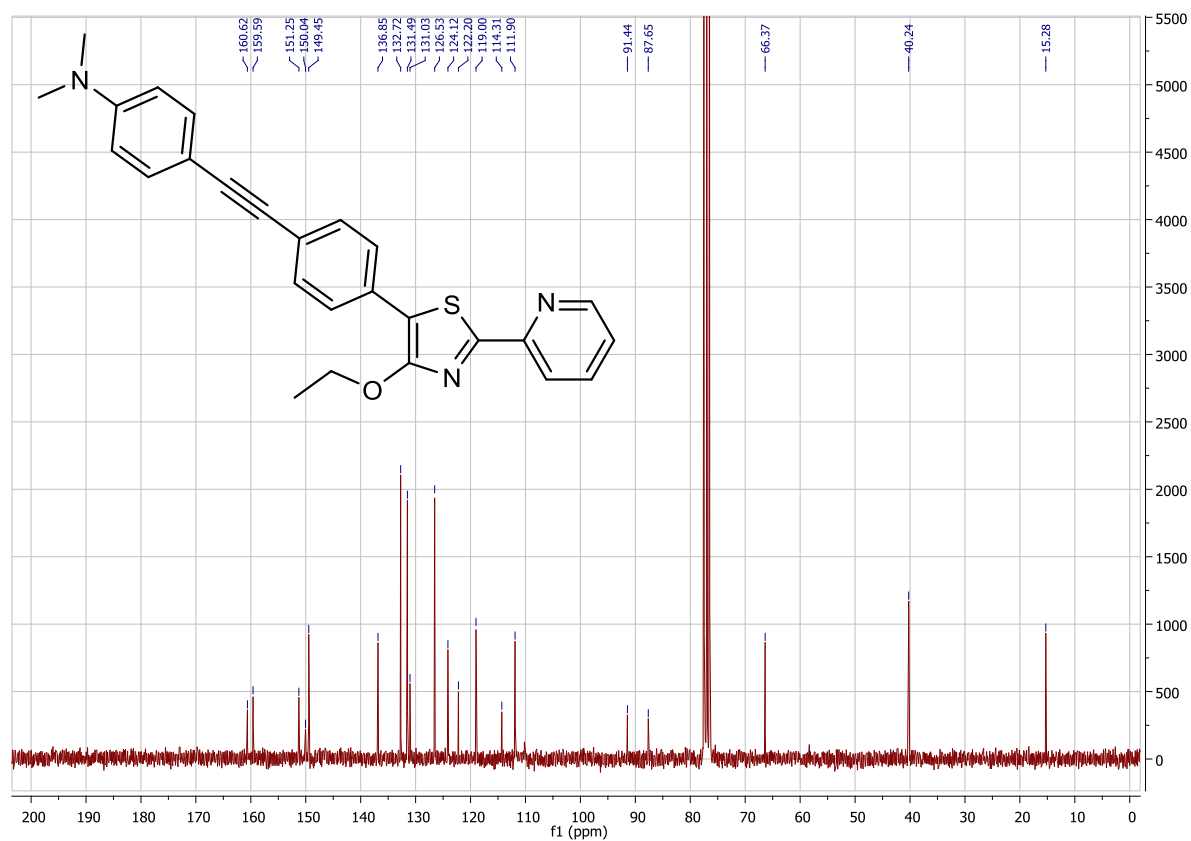
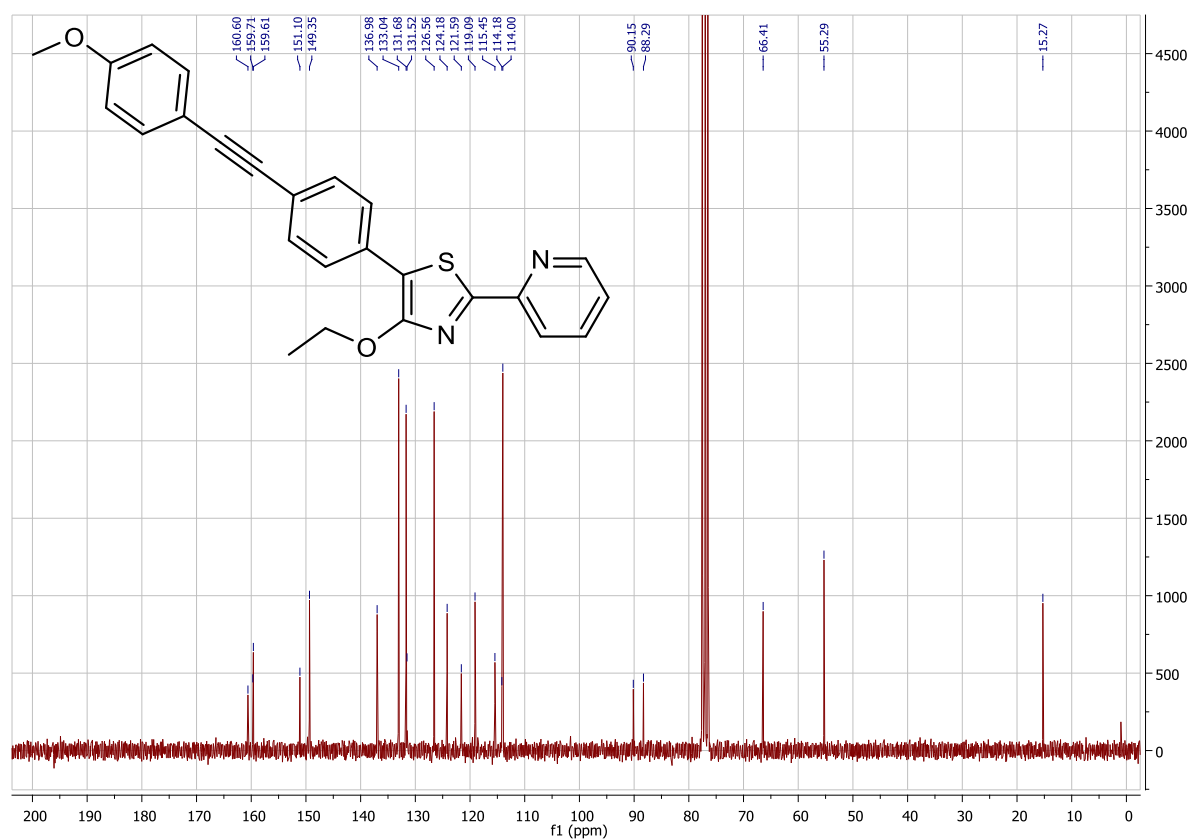
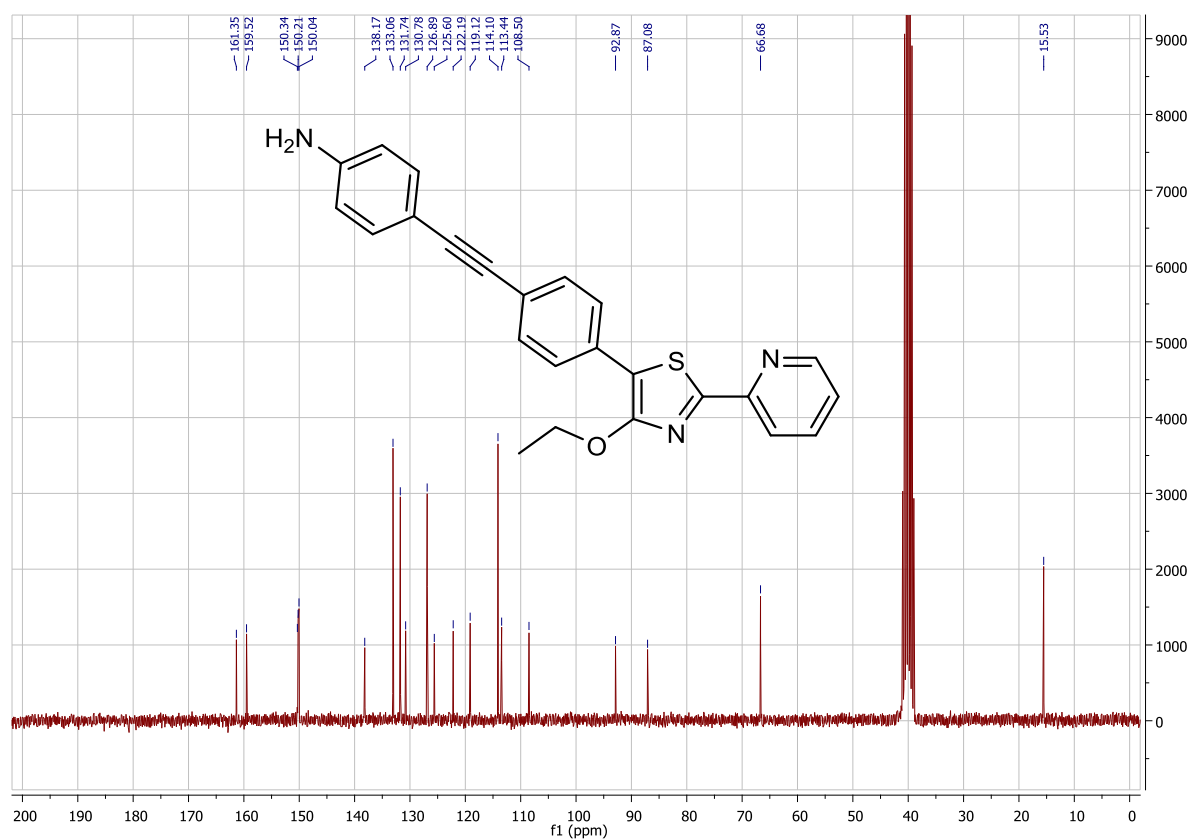
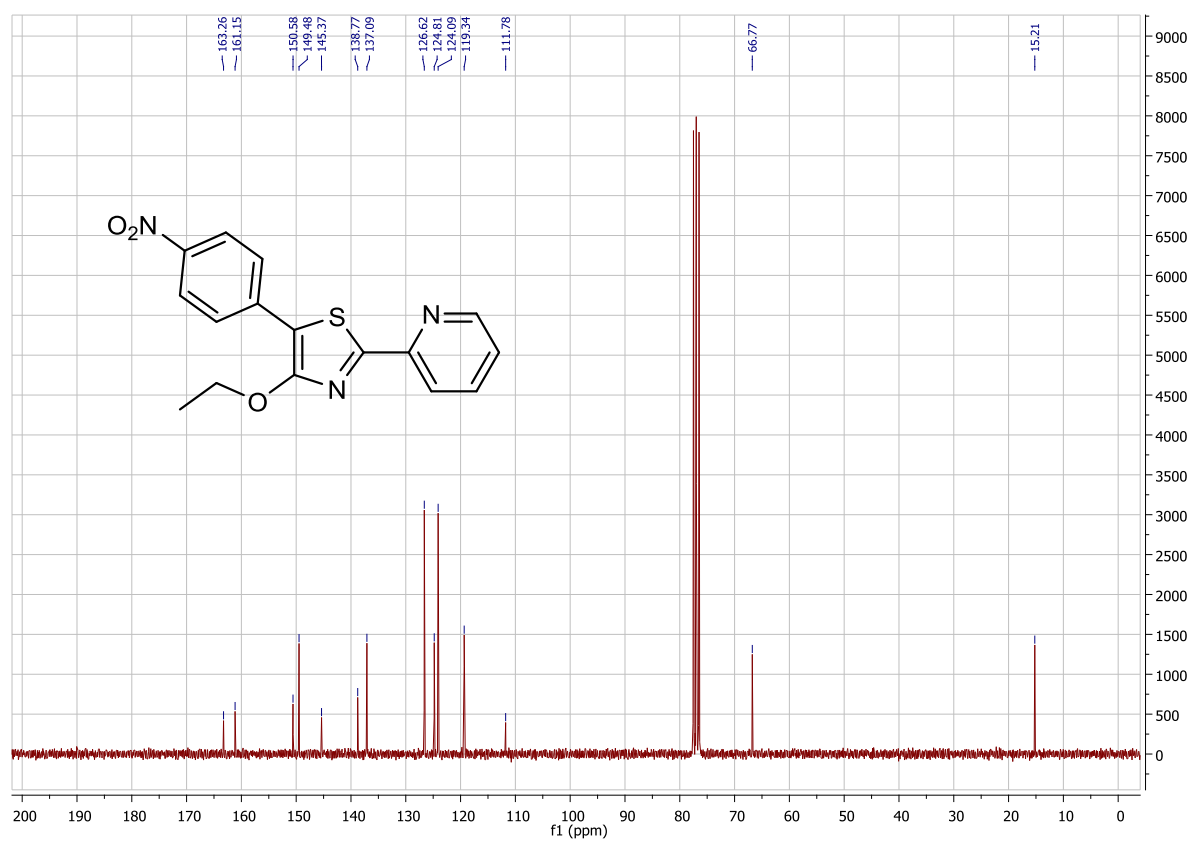
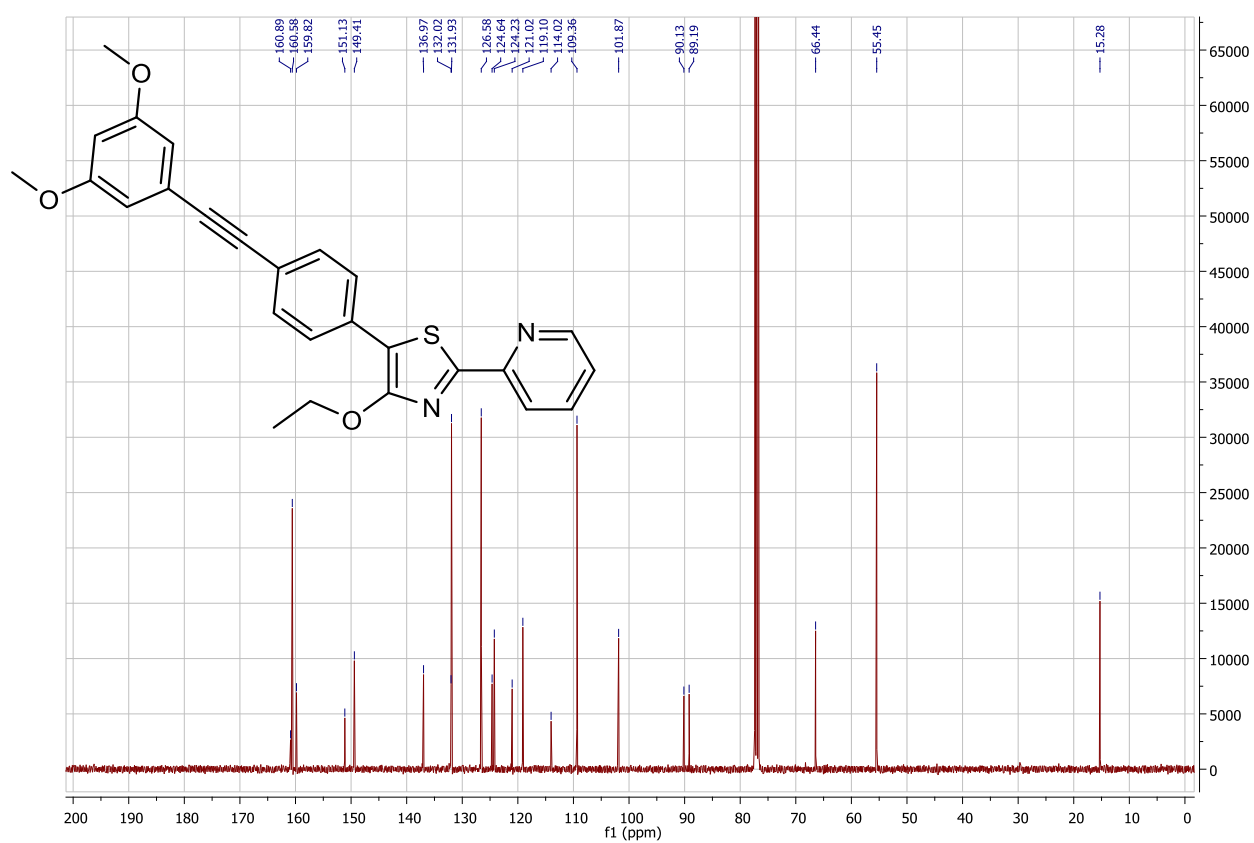


Figure S19: ^{13}C NMR spectrum of 3a.





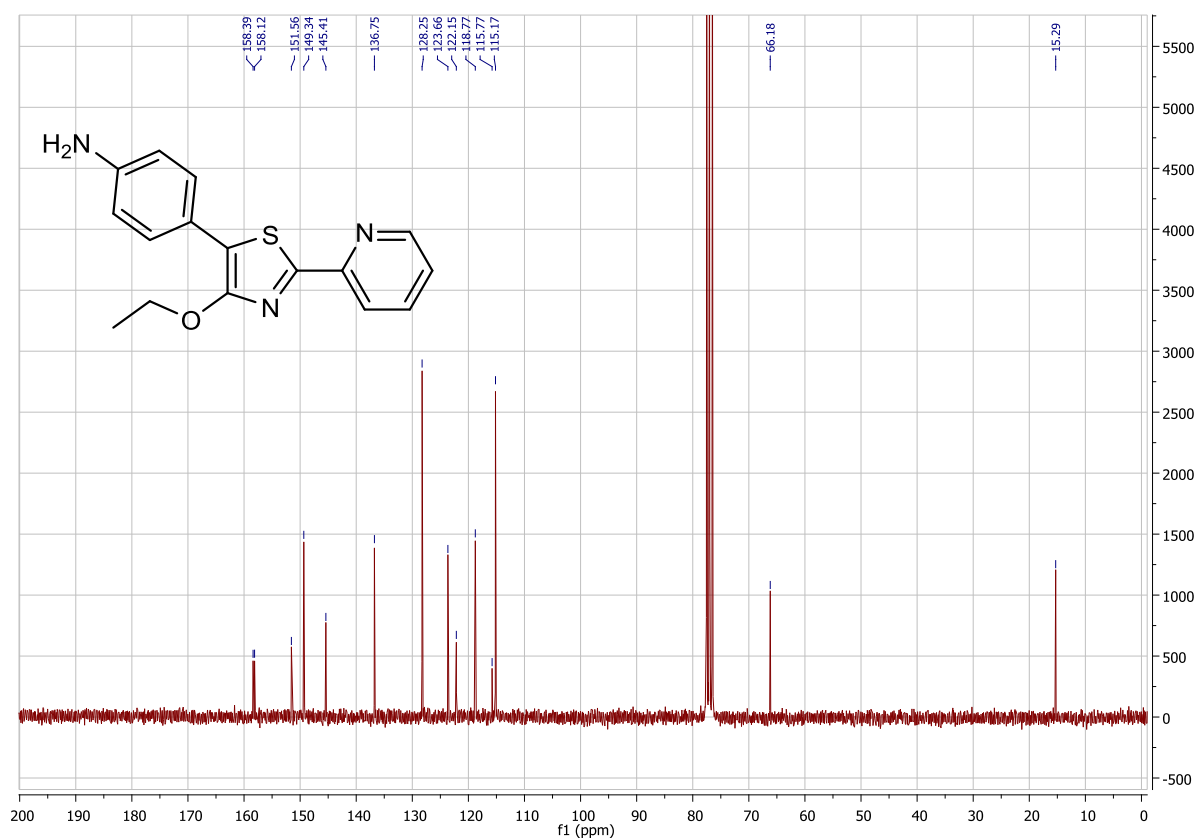


Figure S24: ¹³C NMR spectrum of 6b.

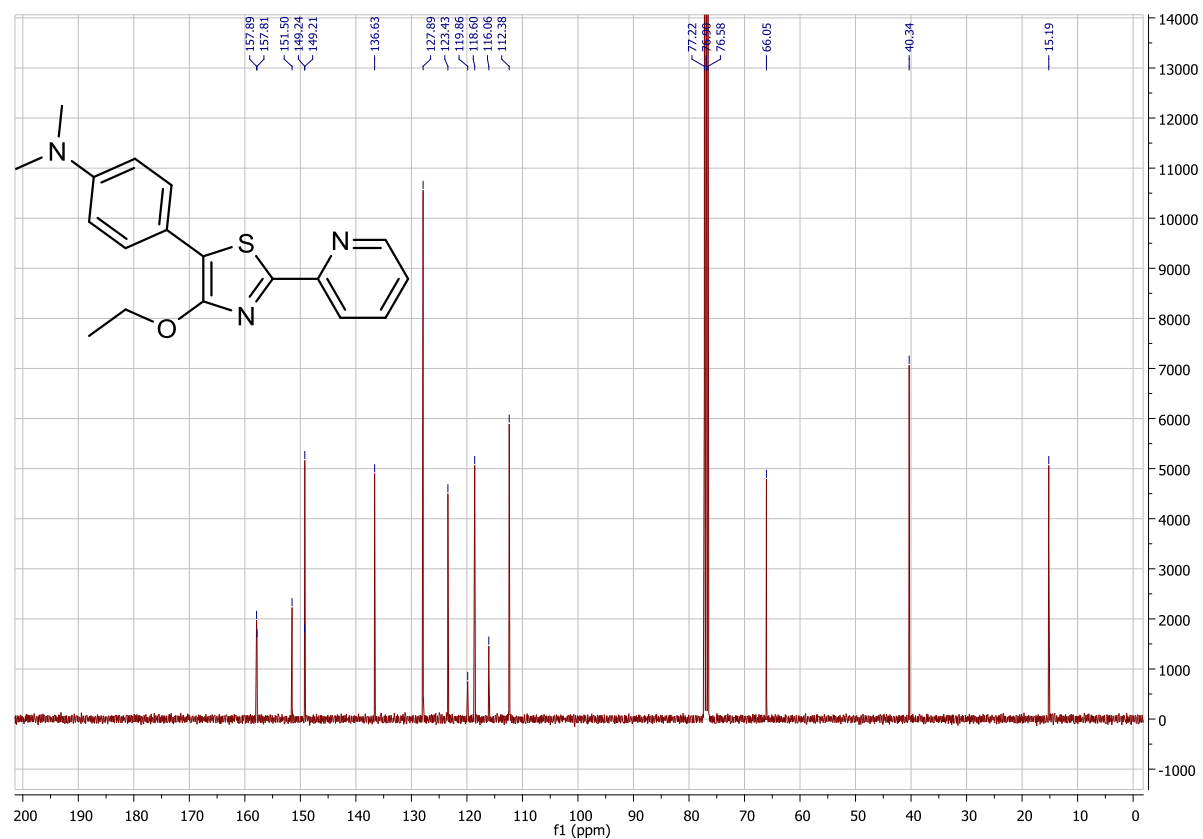


Figure S25: ¹³C NMR spectrum of 6a.

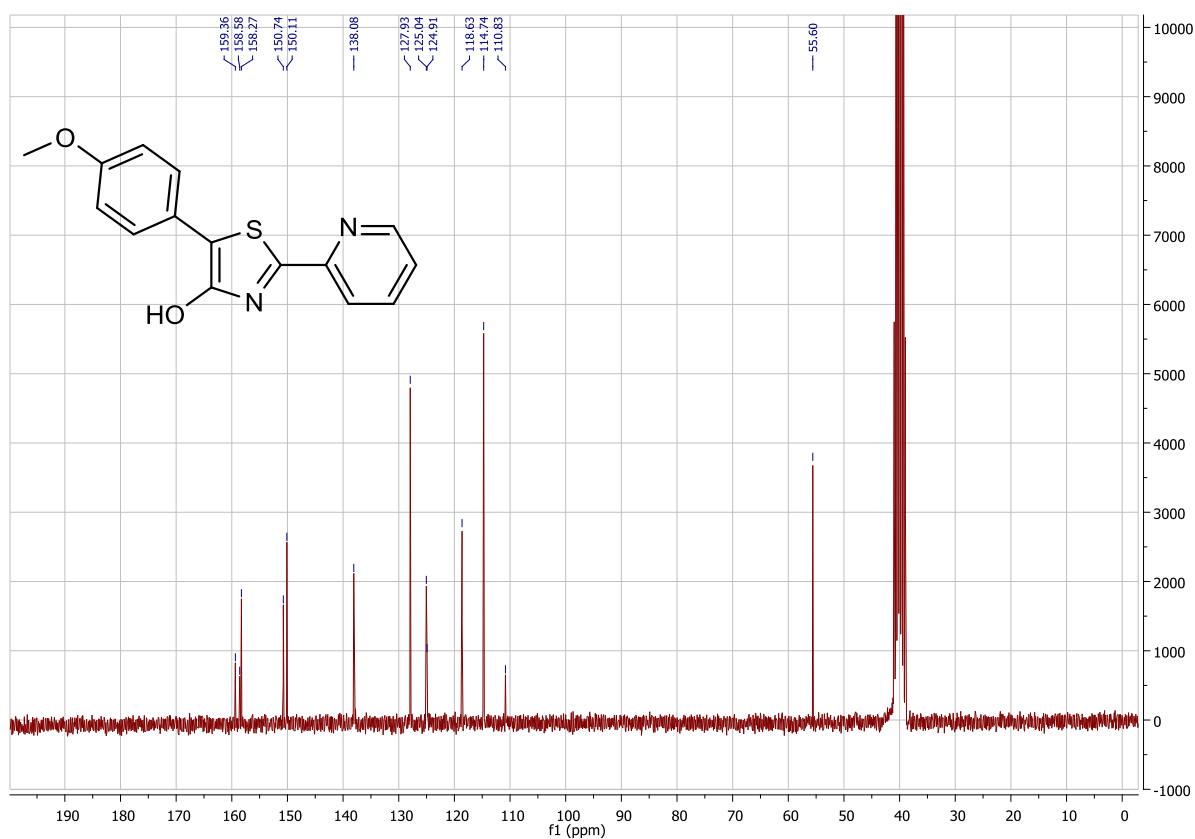


Figure S26: ¹³C NMR spectrum of 9.

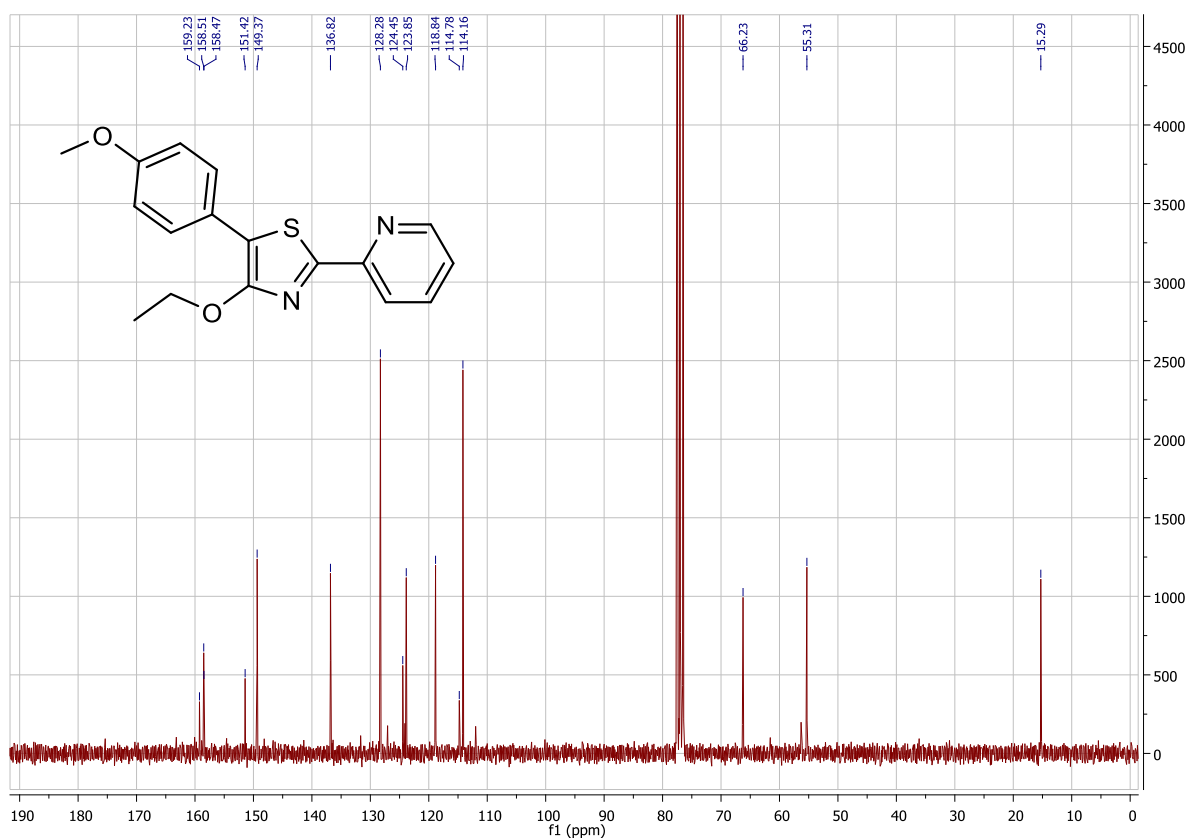


Figure S27: ¹³C NMR spectrum of 6c.