

SUPPORTING INFORMATION

**TBAI/TBHP-Catalyzed [3+2] cycloaddition/oxidation/aromatization cascade and online  
ESI-MS mechanistic studies: Synthesis of pyrrolo[2,1-*a*]isoquinolines and  
indolizino[8,7-*b*]indoles**

Shalini Nekkanti,<sup>a</sup> Niggula Praveen Kumar,<sup>a</sup> Pankaj Sharma,<sup>a</sup> Ahmed Kamal,<sup>a,b</sup> Fabiane M.  
Nachtigall,<sup>c</sup> Oscar Forero-Doria,<sup>d</sup> Leonardo S. Santos,<sup>c,d\*</sup> Nagula Shankaraiah<sup>a\*</sup>

<sup>a</sup>*Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and  
Research (NIPER), Hyderabad 500 037, India*

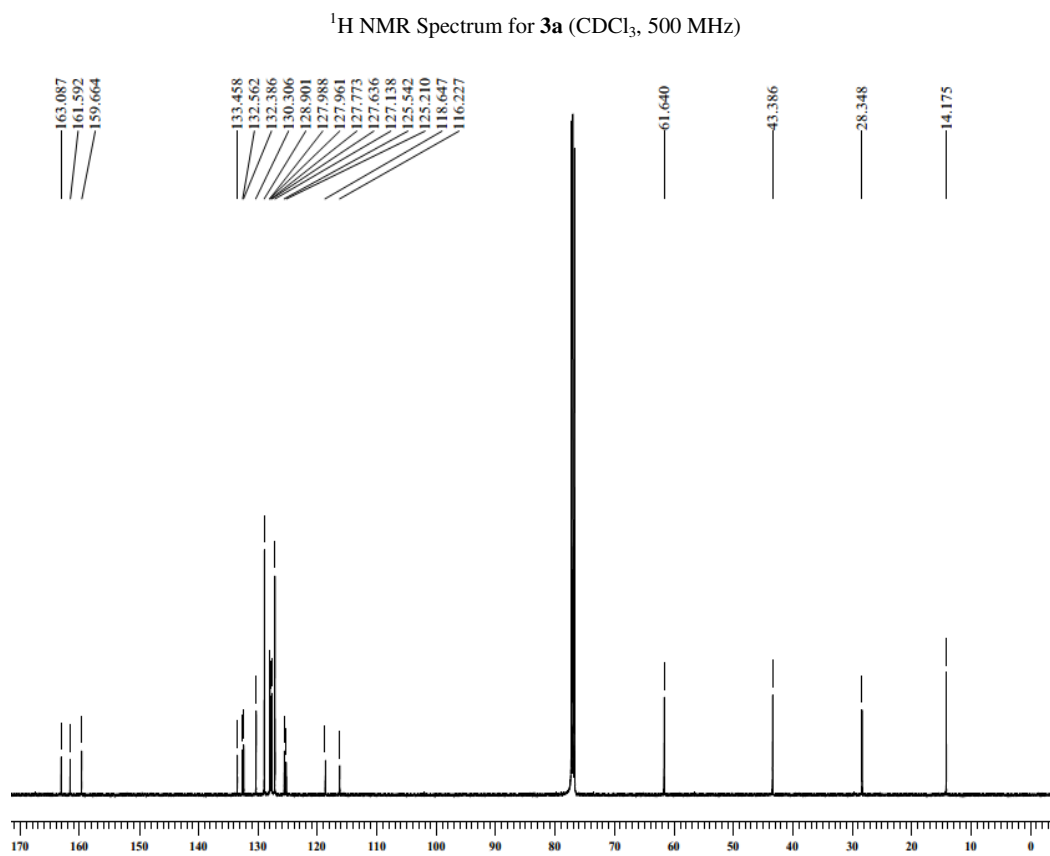
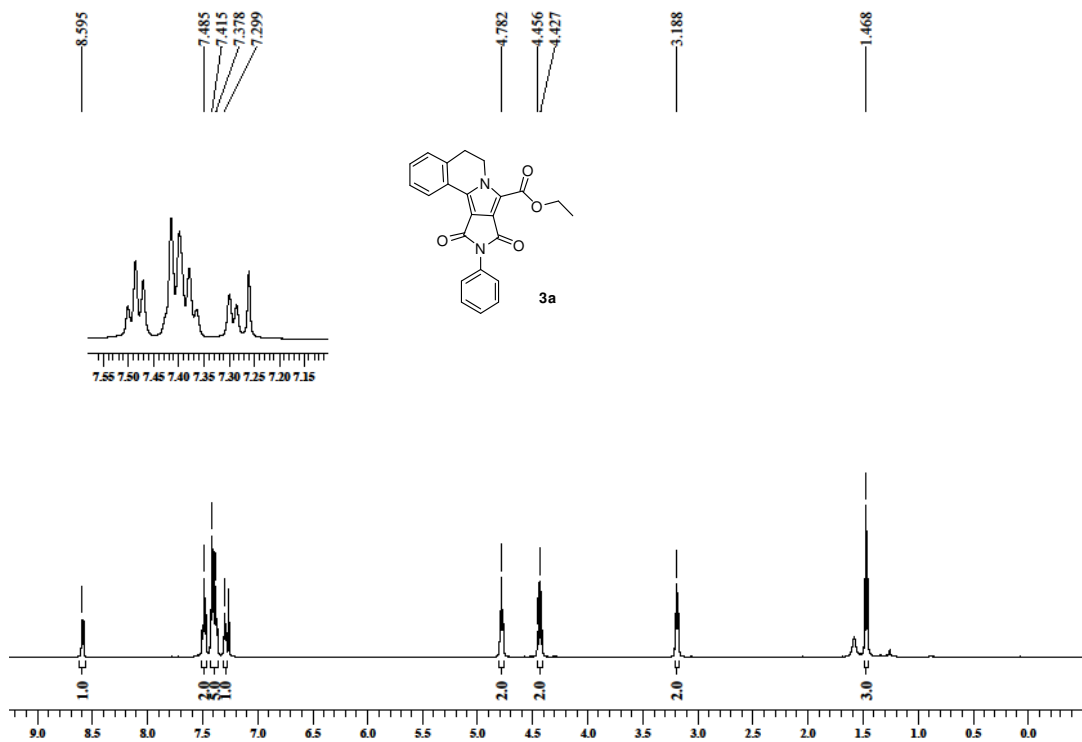
<sup>b</sup>*Medicinal Chemistry & Pharmacology, CSIR-Indian Institute of Chemical Technology,  
Hyderabad 500 007, India*

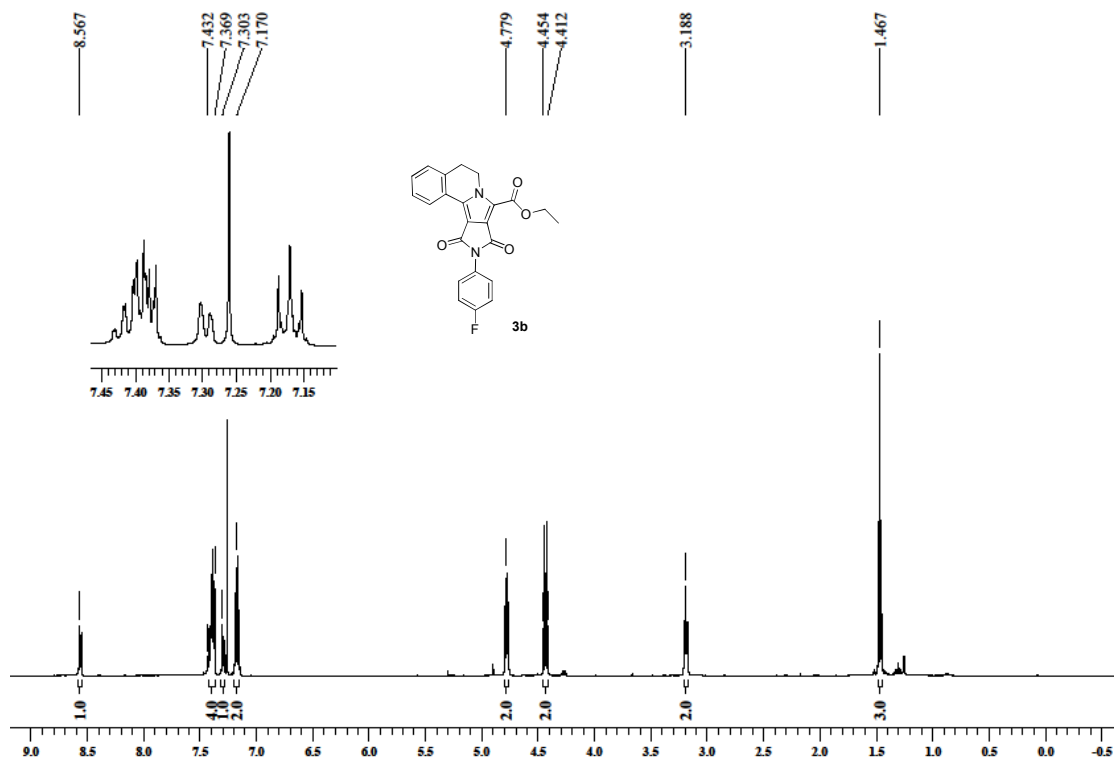
<sup>c</sup>*Fraunhofer Chile Research Foundation-Center System Biotechnology, FCR-CSB,  
Nanobiotechnology Division at University of Talca, P.O. Box 747, Talca, Chile*

<sup>d</sup>*Laboratory of Asymmetric Synthesis, Chemistry Institute of Natural Resources, University  
of Talca, P.O. Box 747, Talca, Chile*

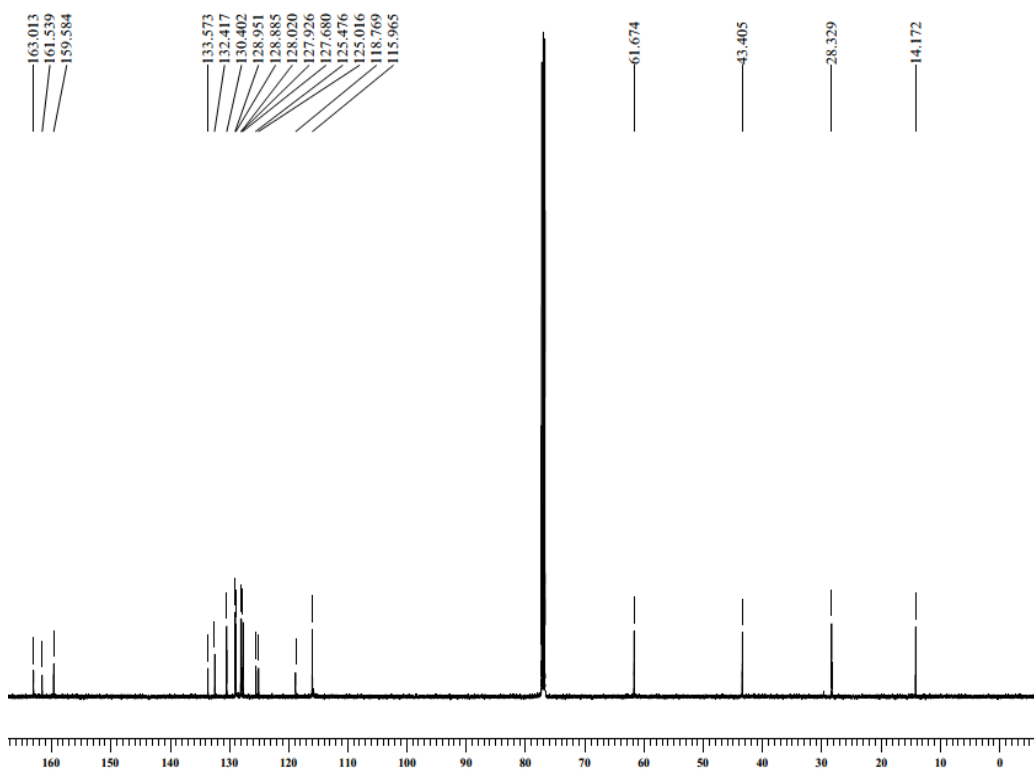
**Table of Contents**

NMR spectra.....S2

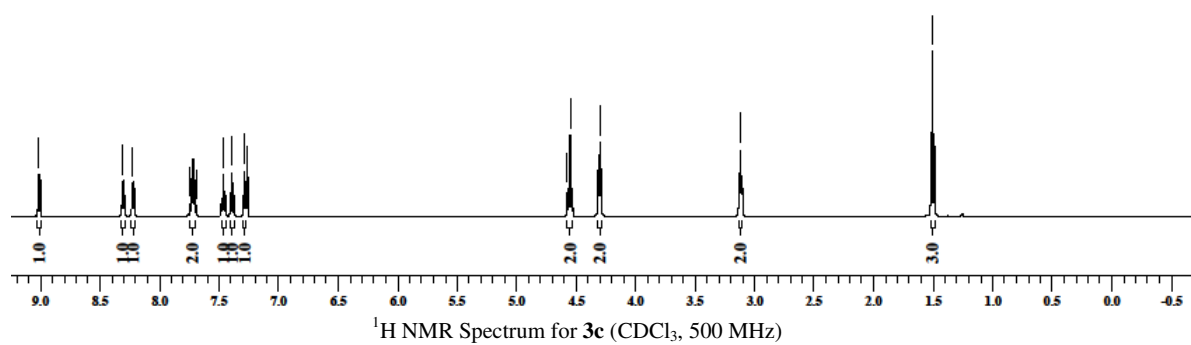
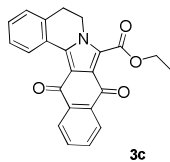
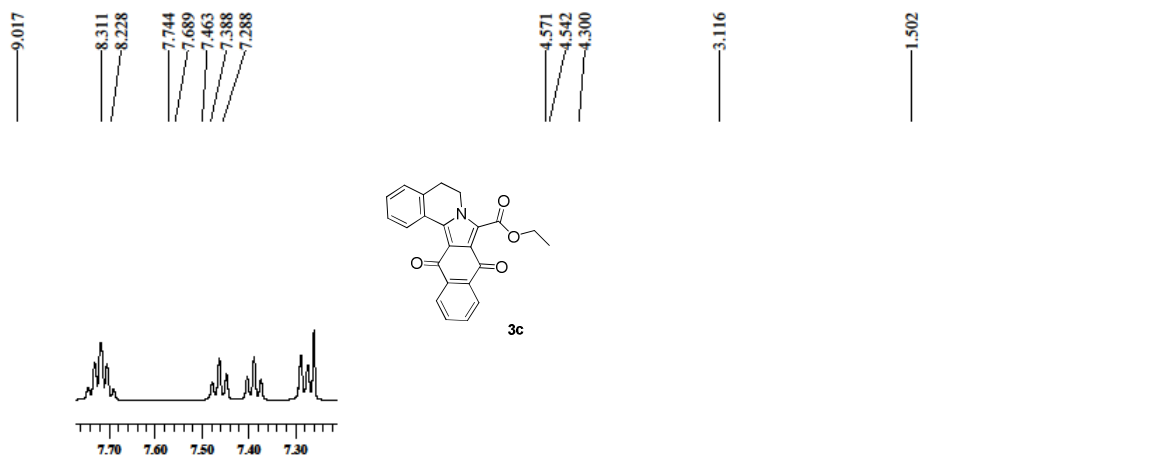


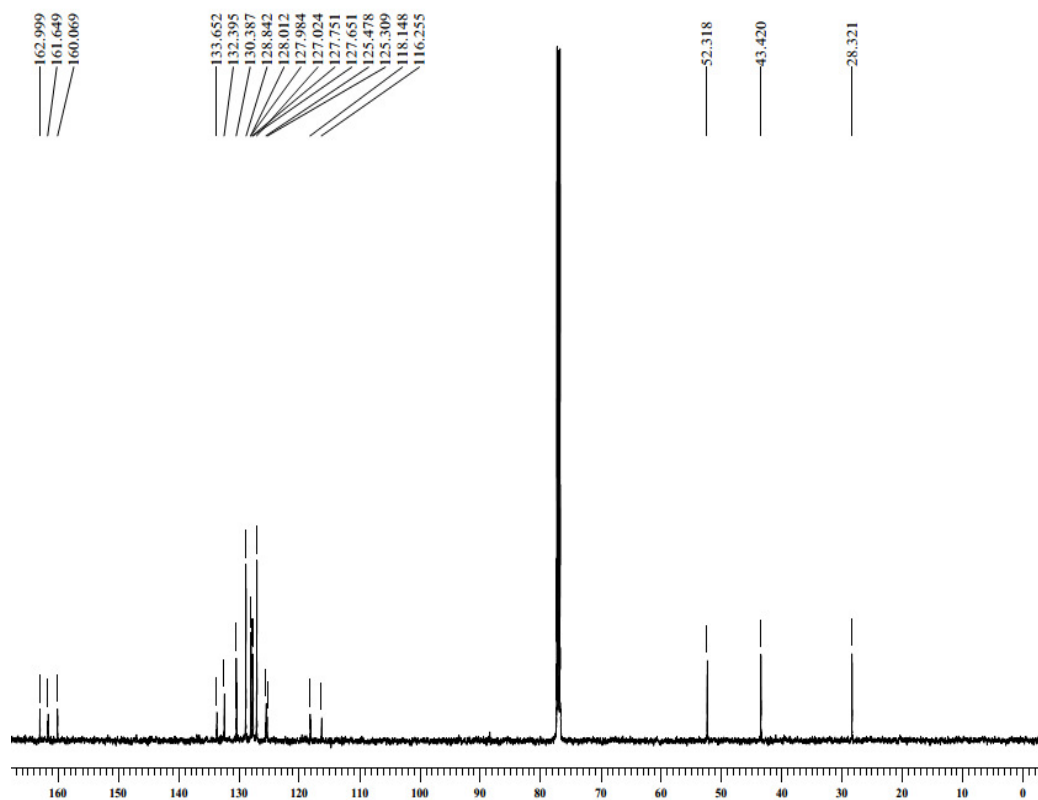
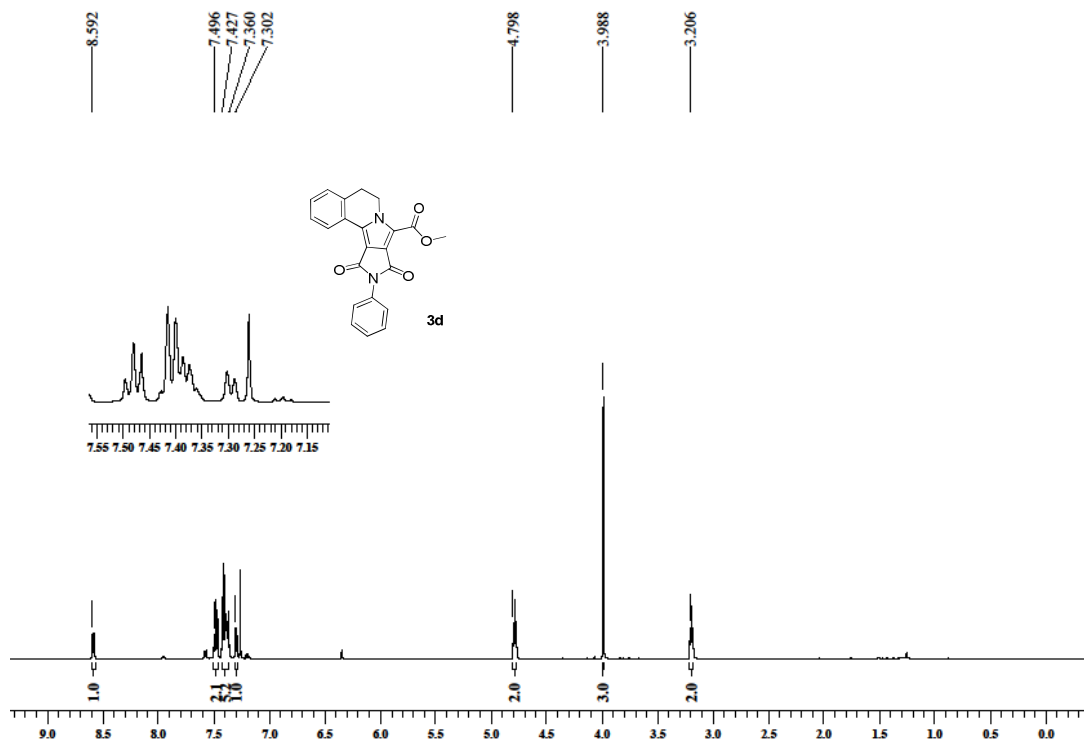


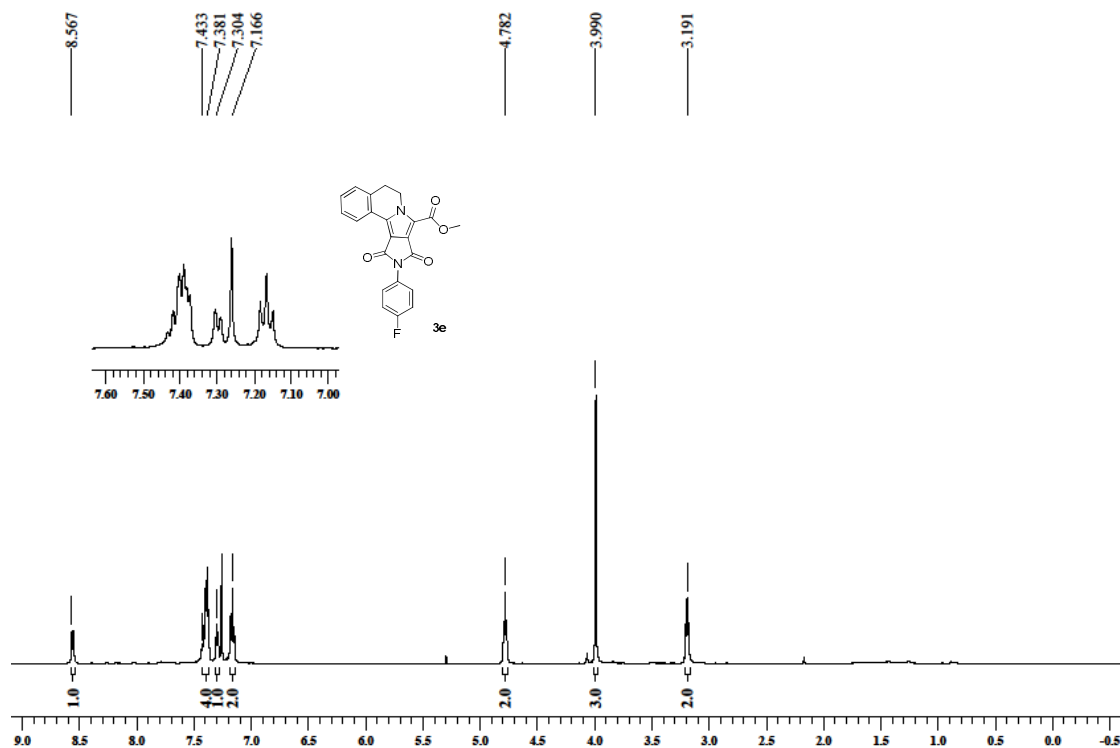
<sup>1</sup>H NMR Spectrum for **3b** (CDCl<sub>3</sub>, 500 MHz)



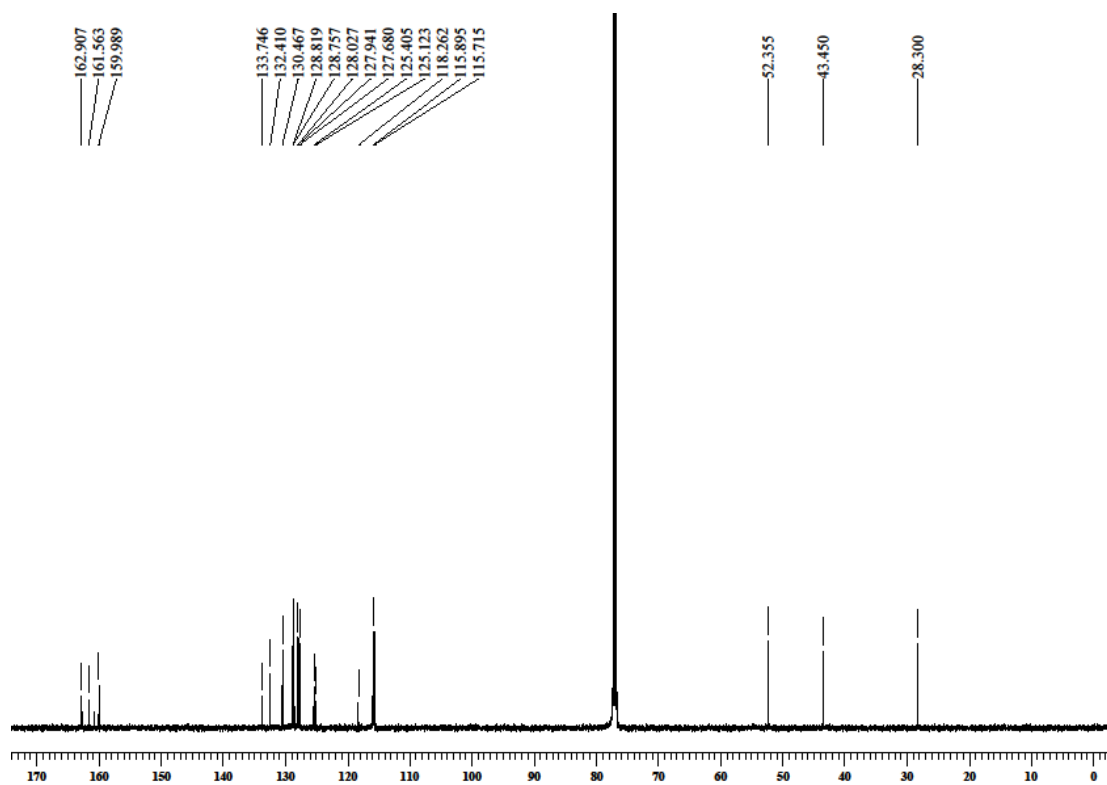
<sup>13</sup>C NMR Spectrum for **3b** (CDCl<sub>3</sub>, 125 MHz)



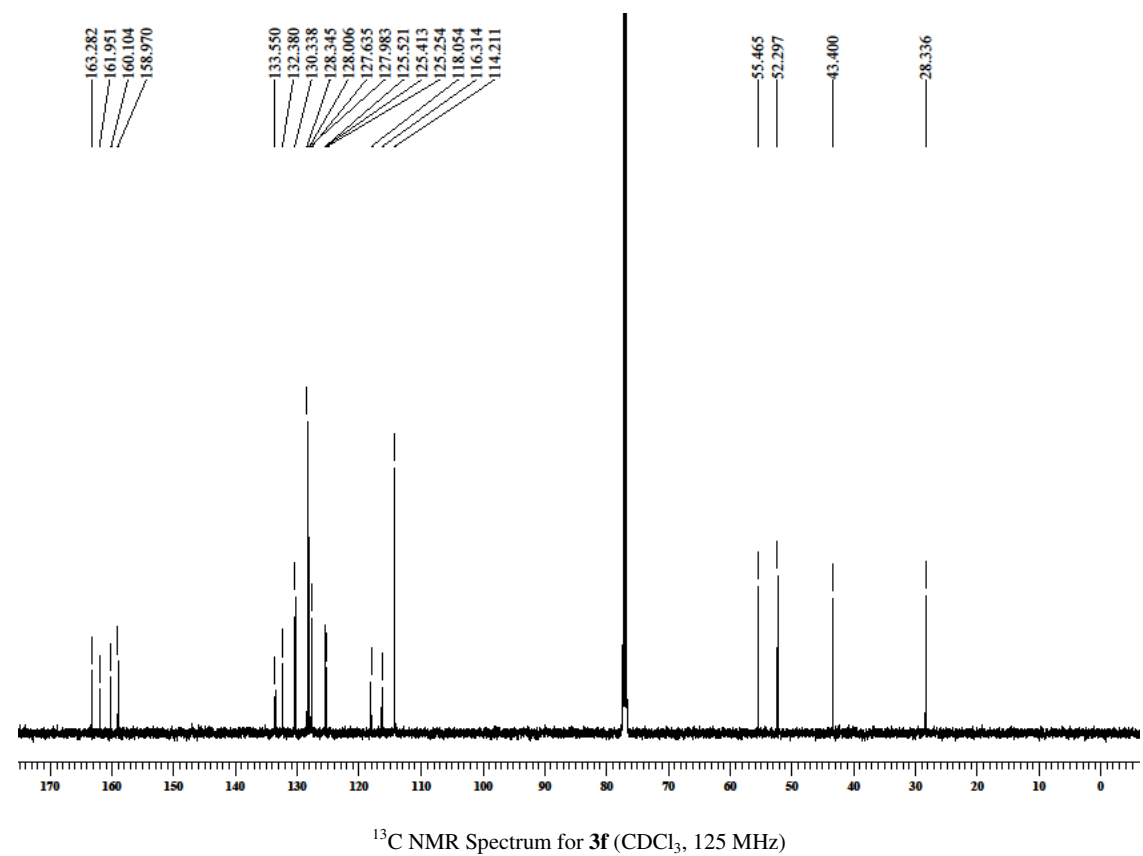
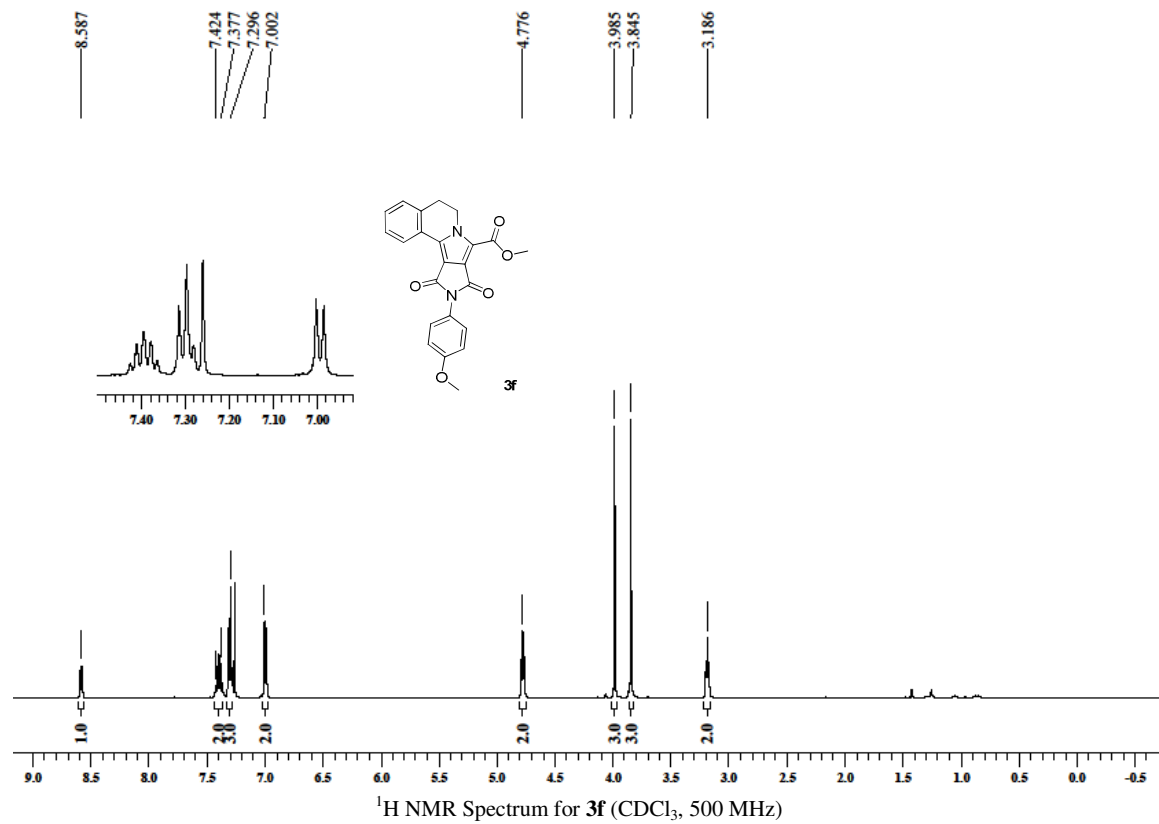


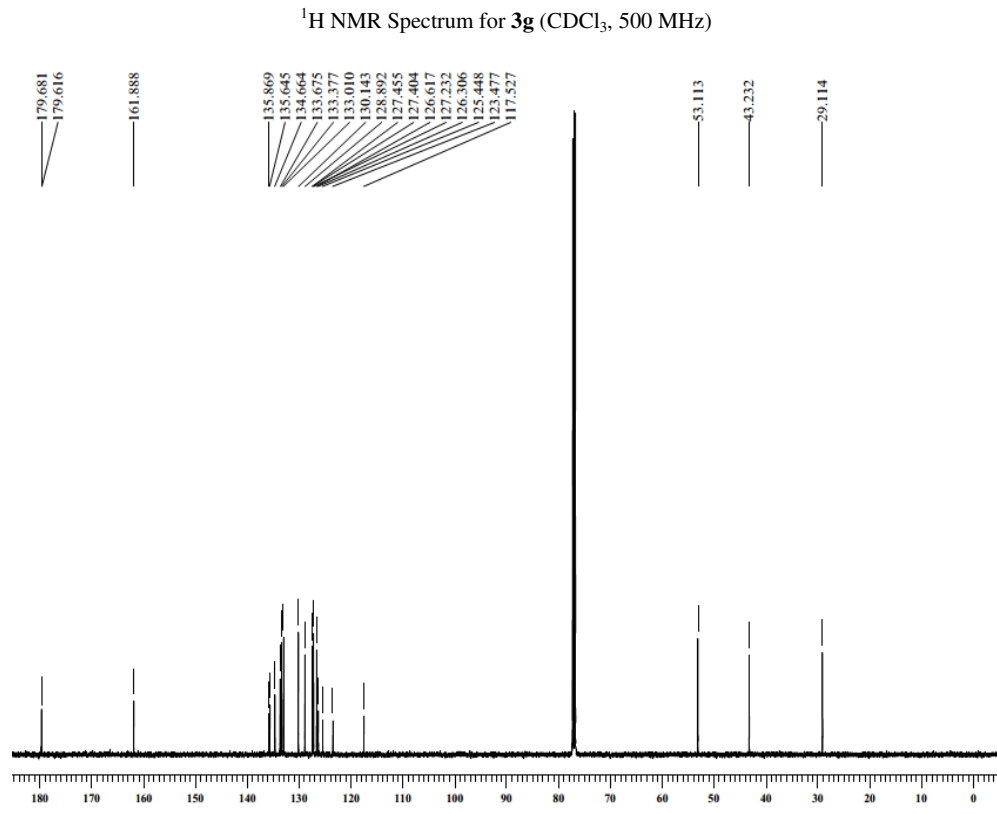
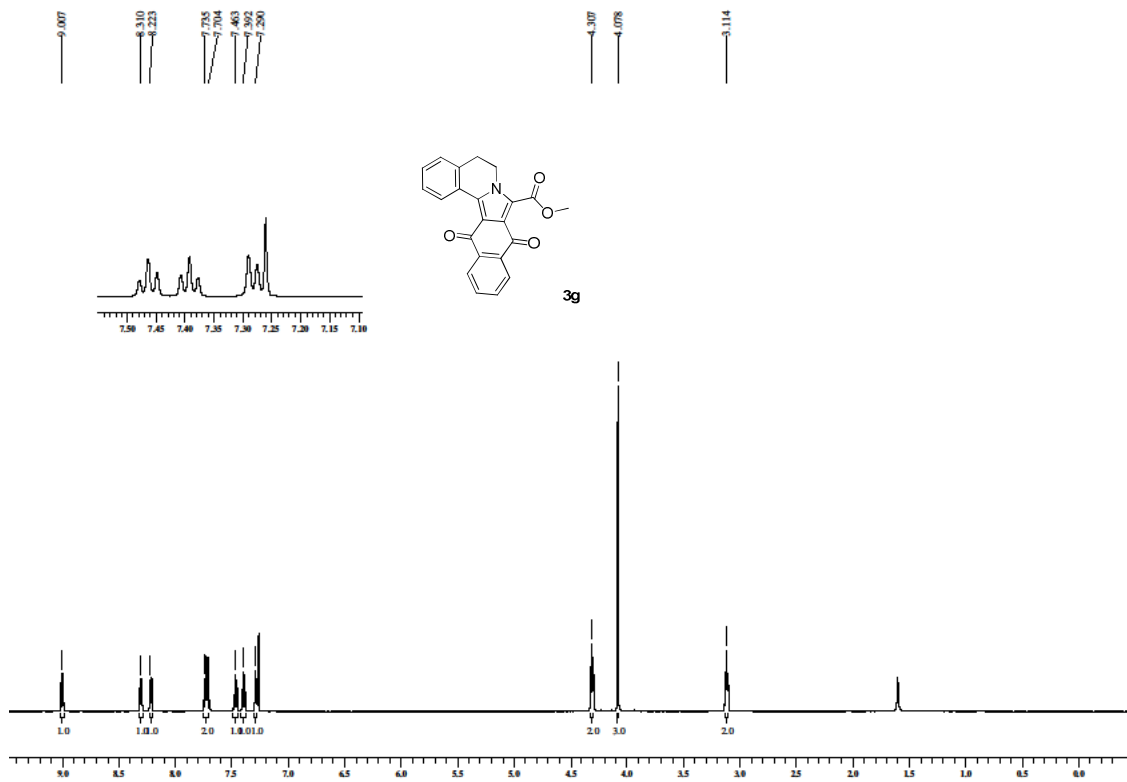


<sup>1</sup>H NMR Spectrum for **3e** (CDCl<sub>3</sub>, 500 MHz)

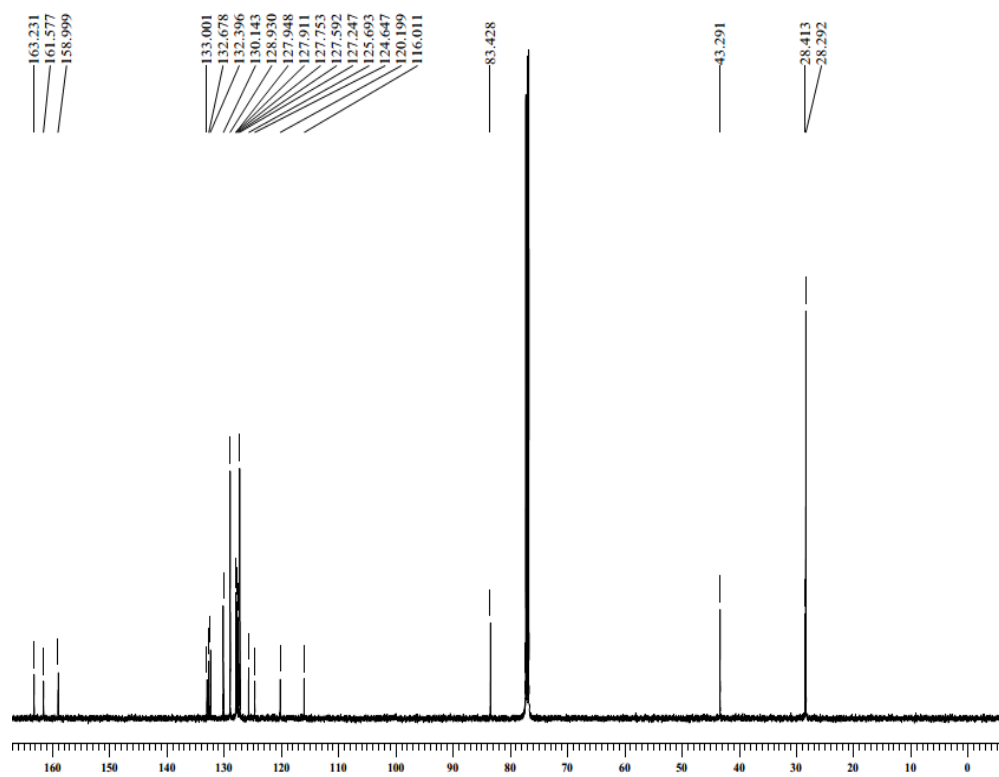
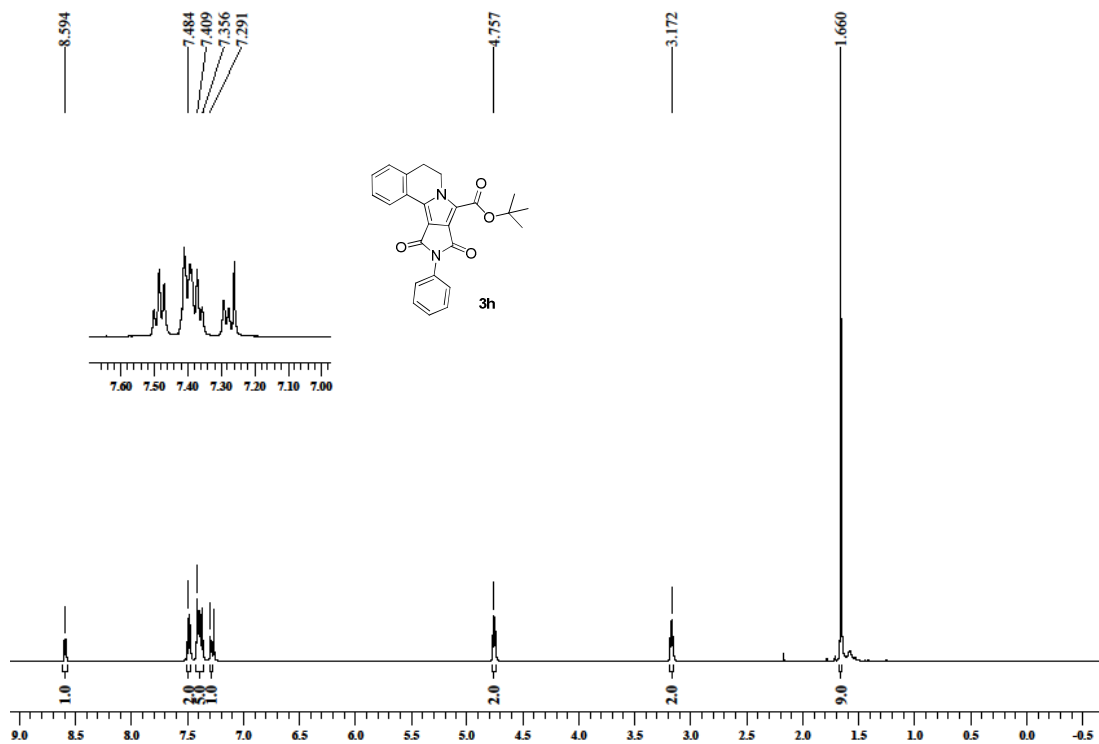


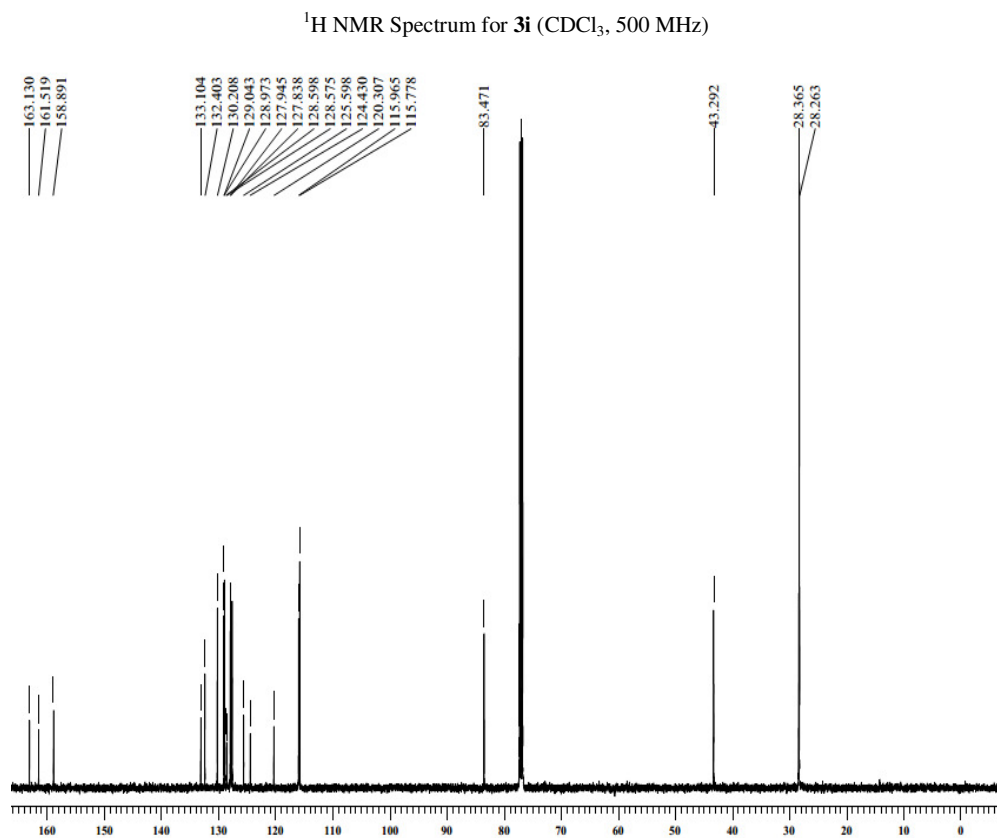
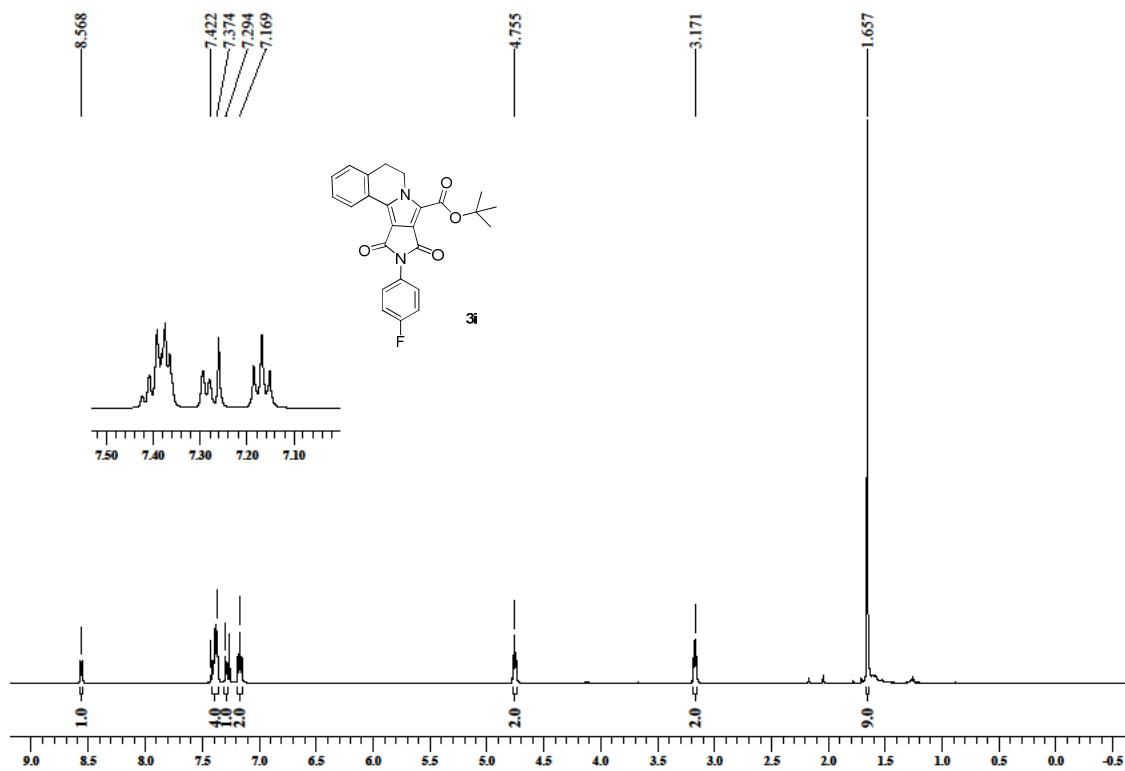
<sup>13</sup>C NMR Spectrum for **3e** (CDCl<sub>3</sub>, 125 MHz)

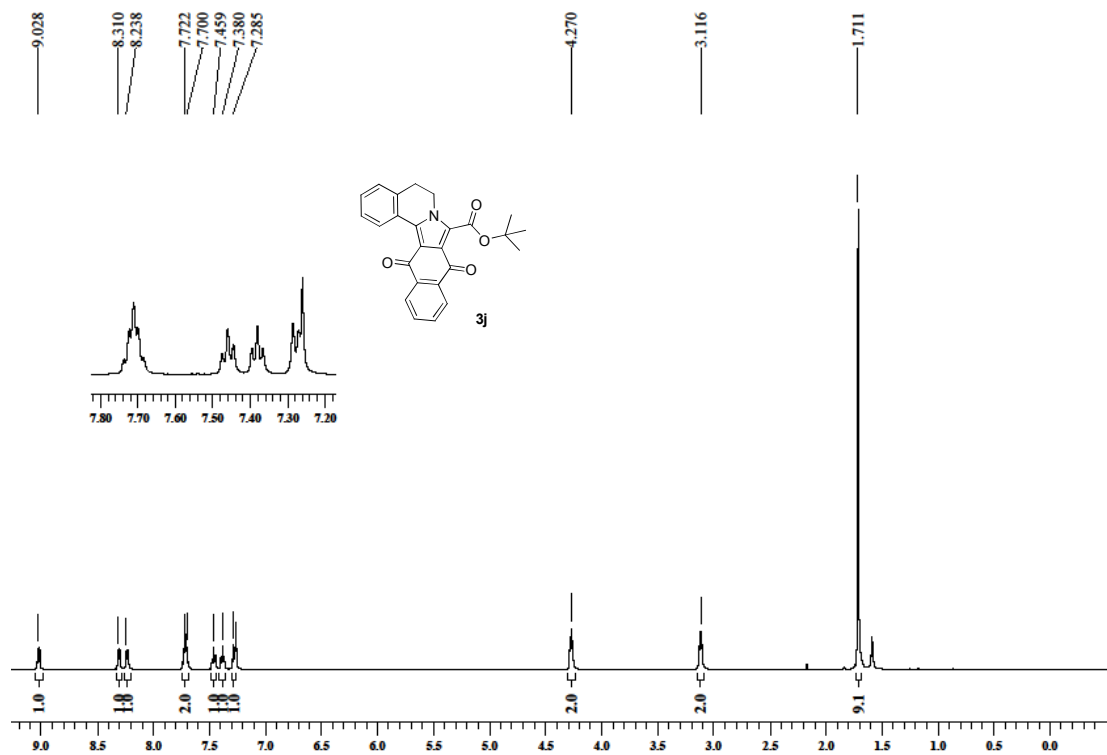




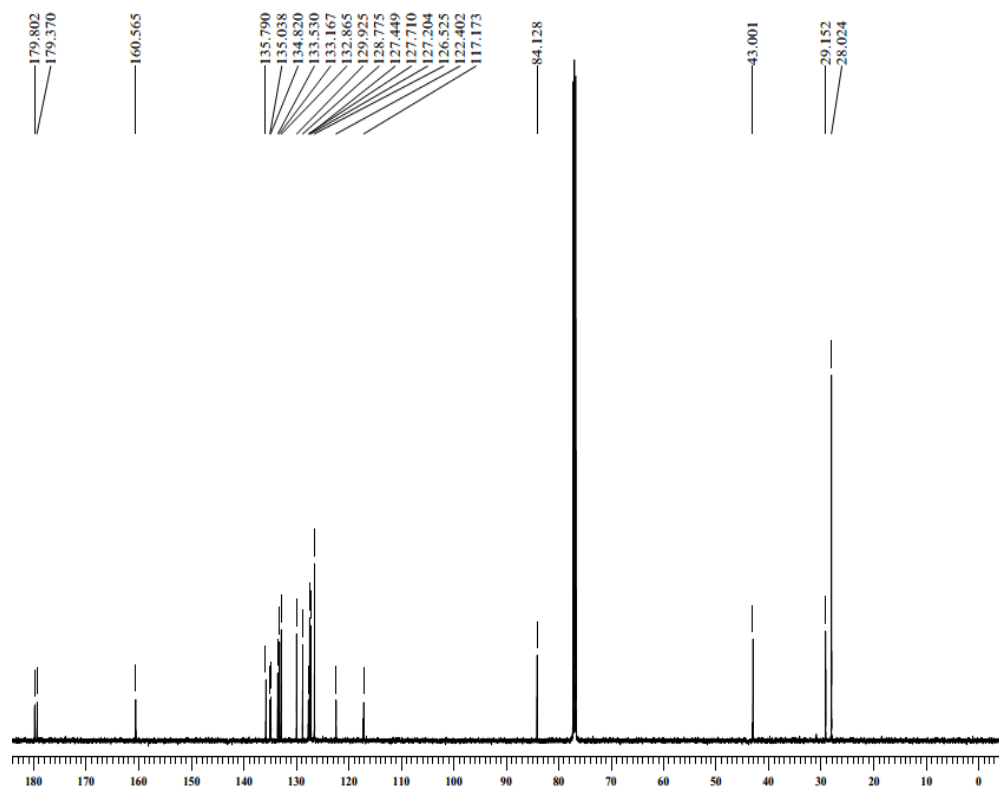




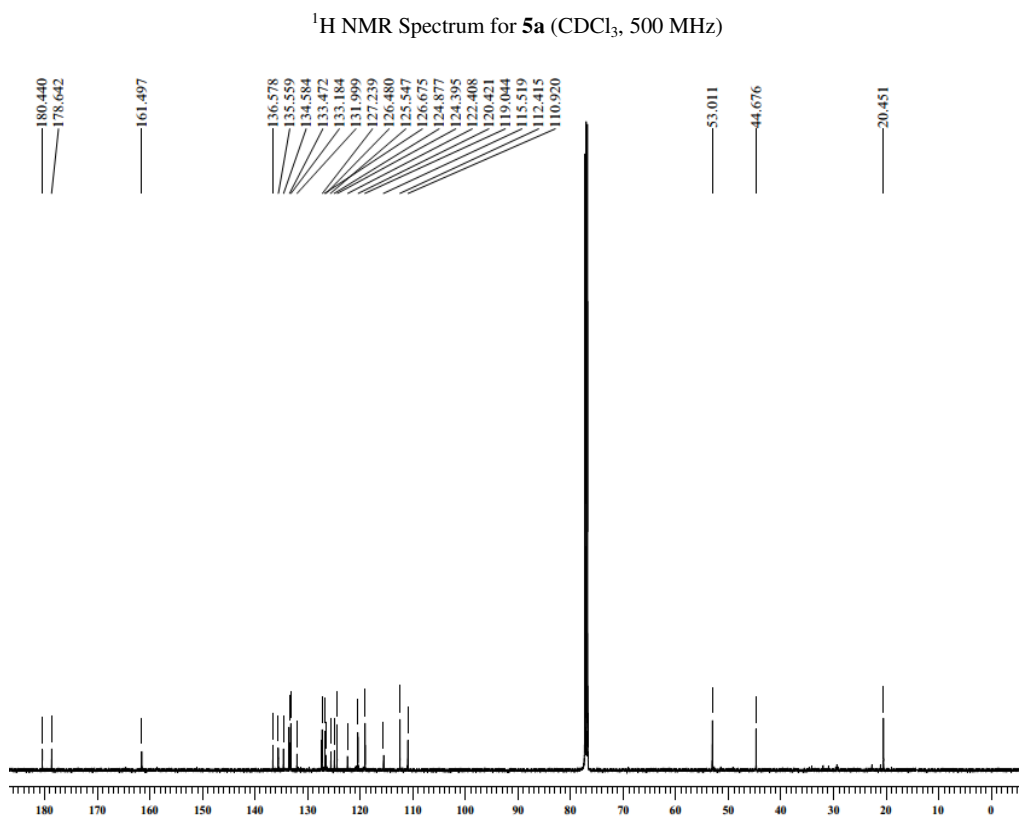
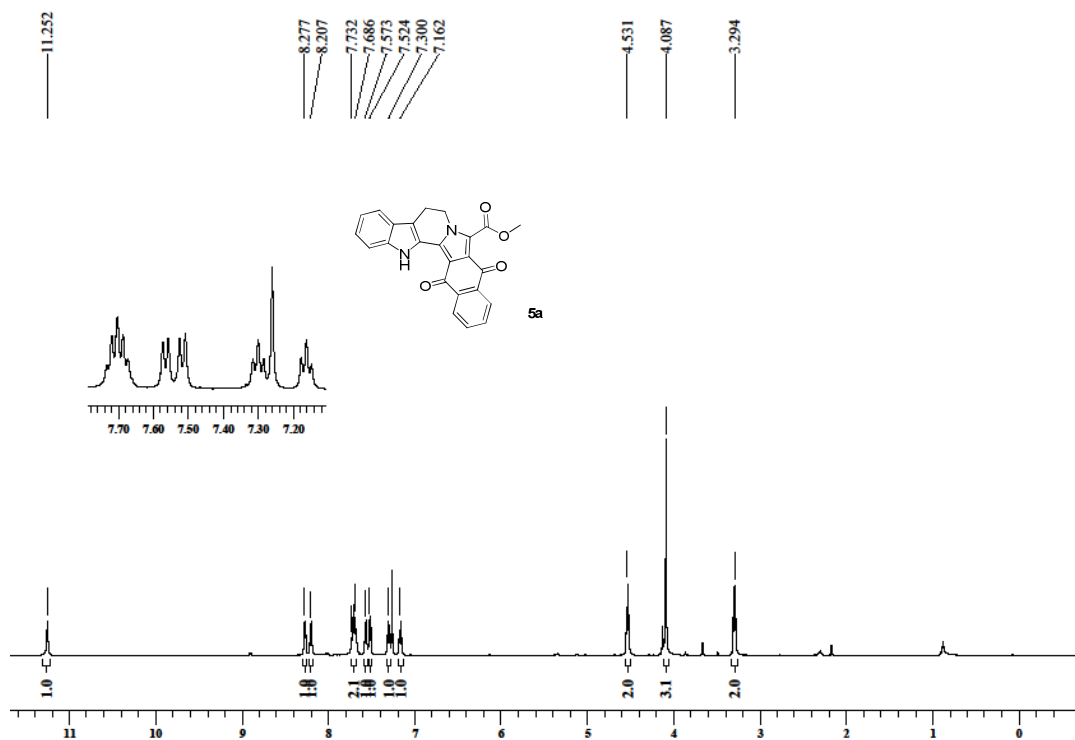


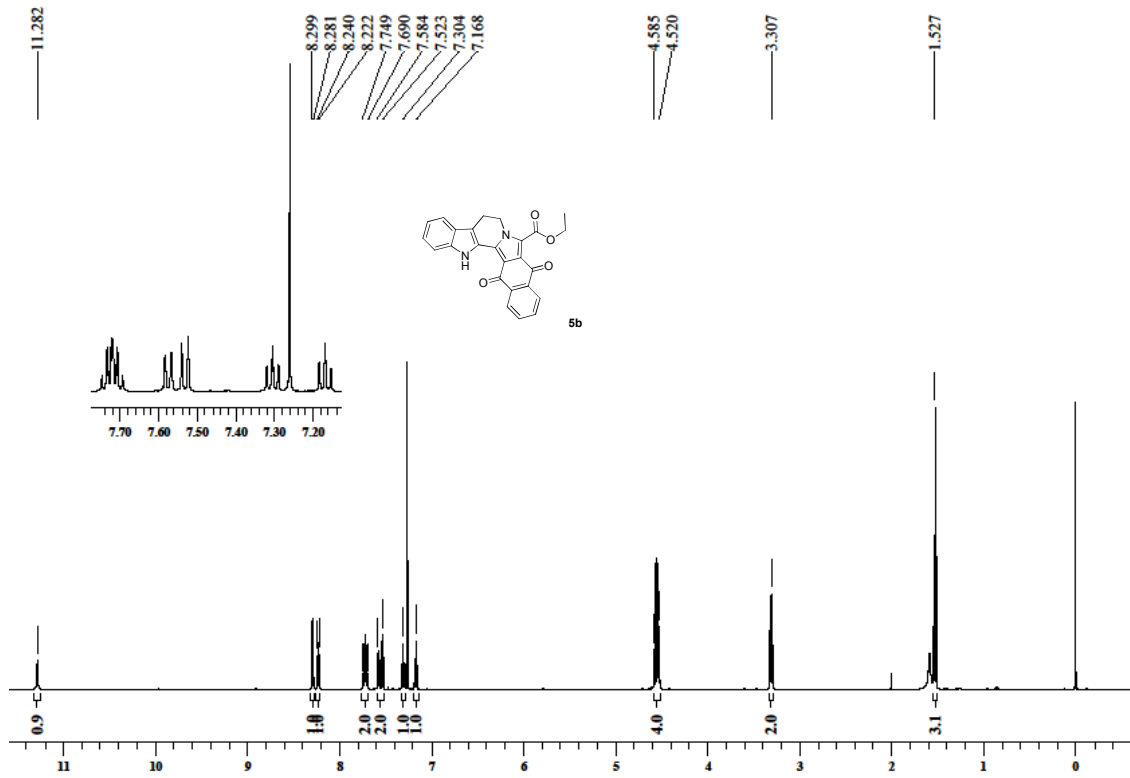


<sup>1</sup>H NMR Spectrum for 3j (CDCl<sub>3</sub>, 500 MHz)

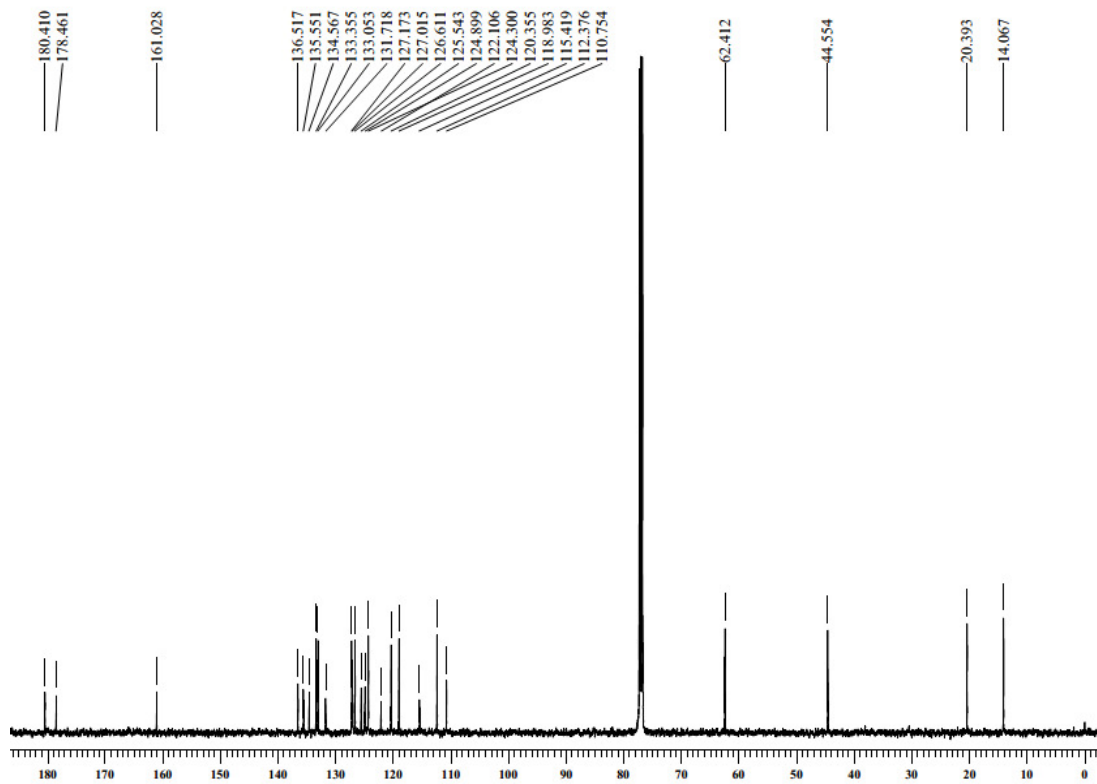


<sup>13</sup>C NMR Spectrum for 3j (CDCl<sub>3</sub>, 125 MHz)

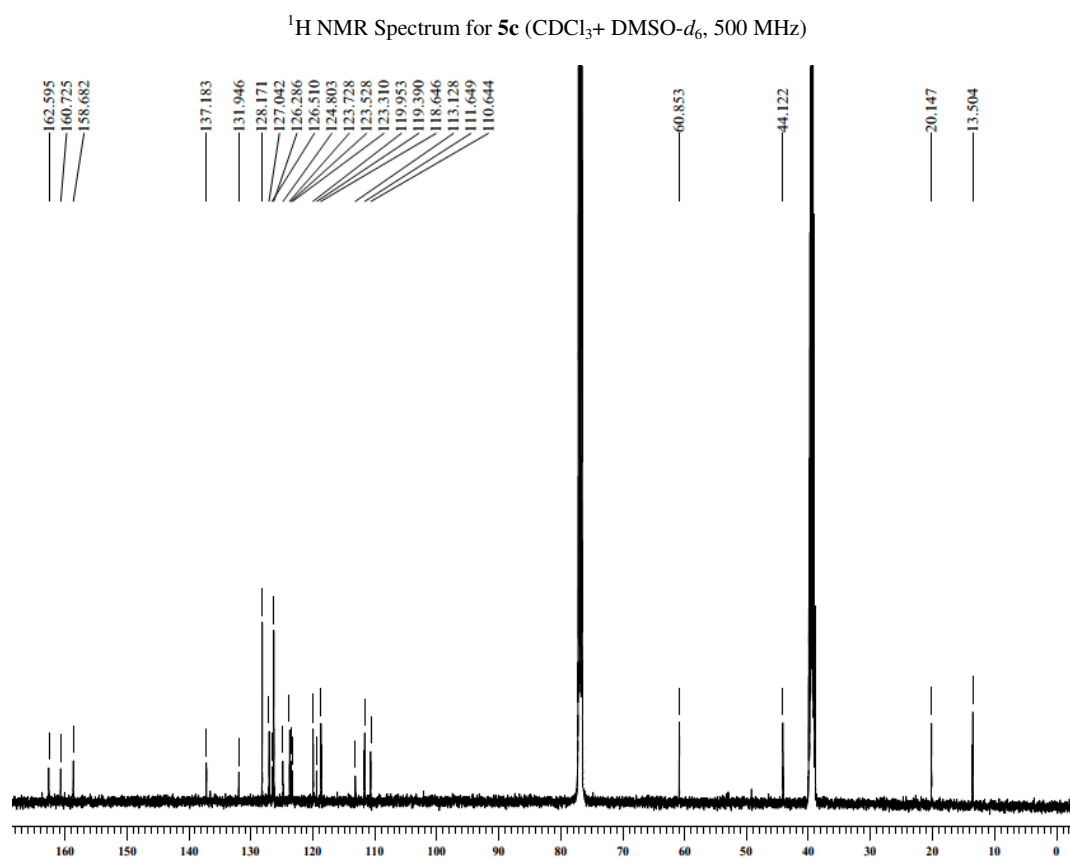
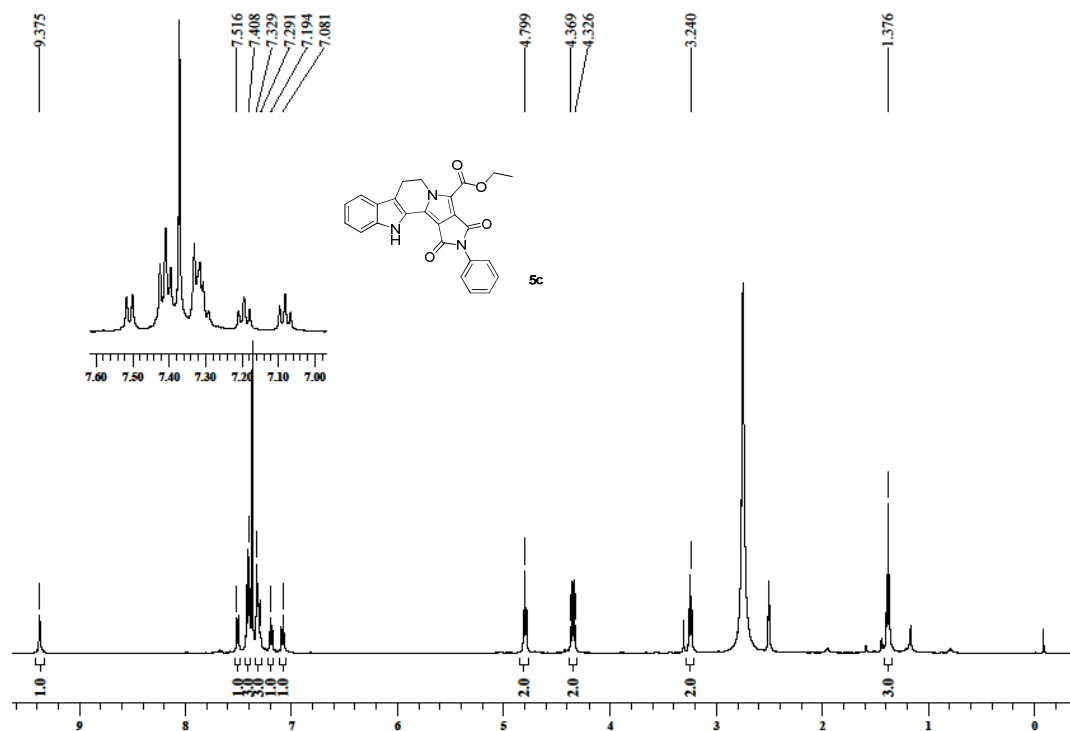


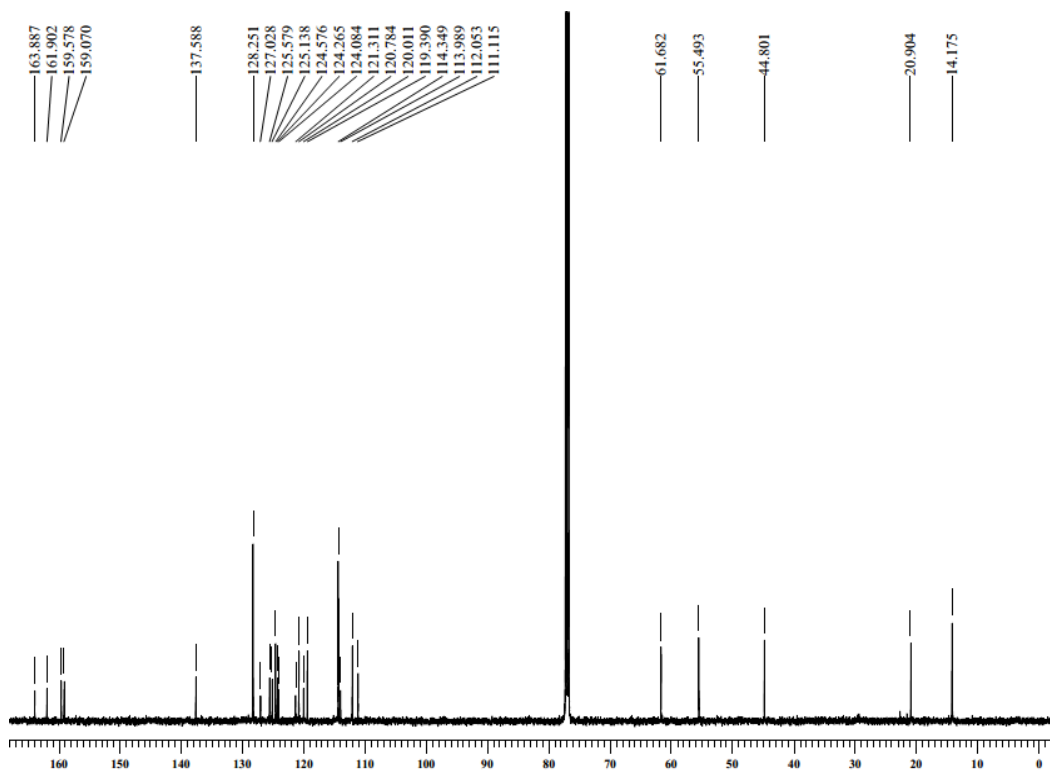
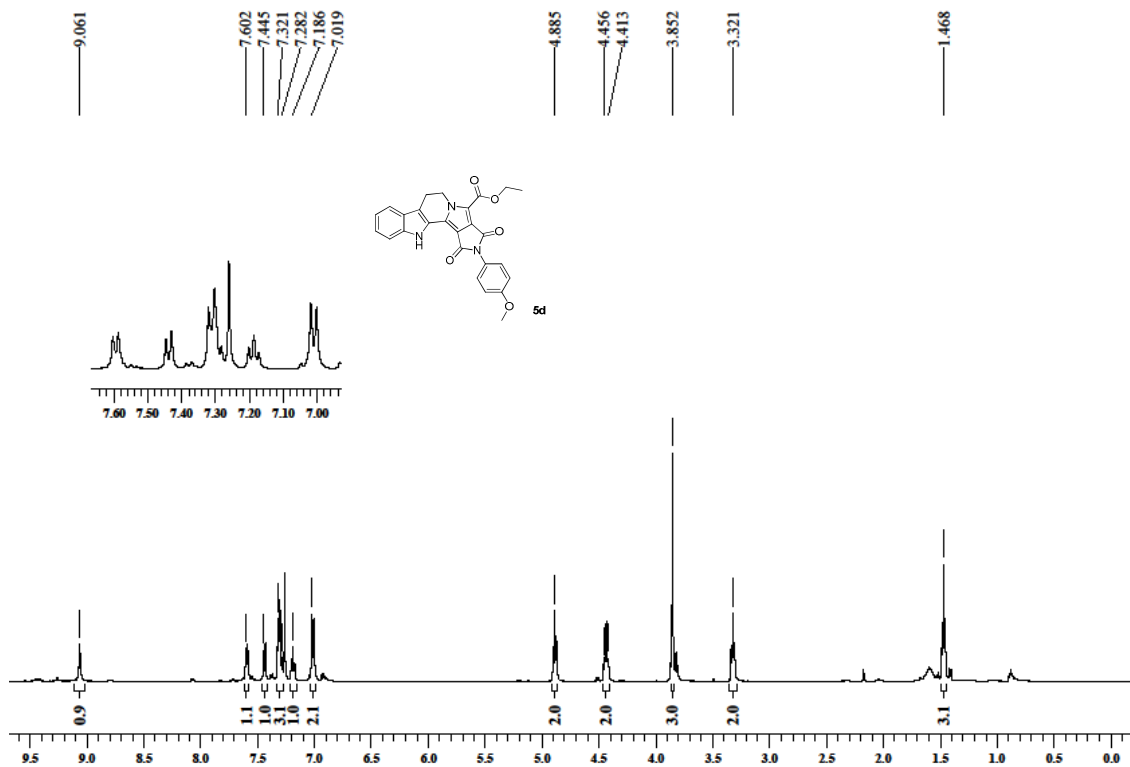


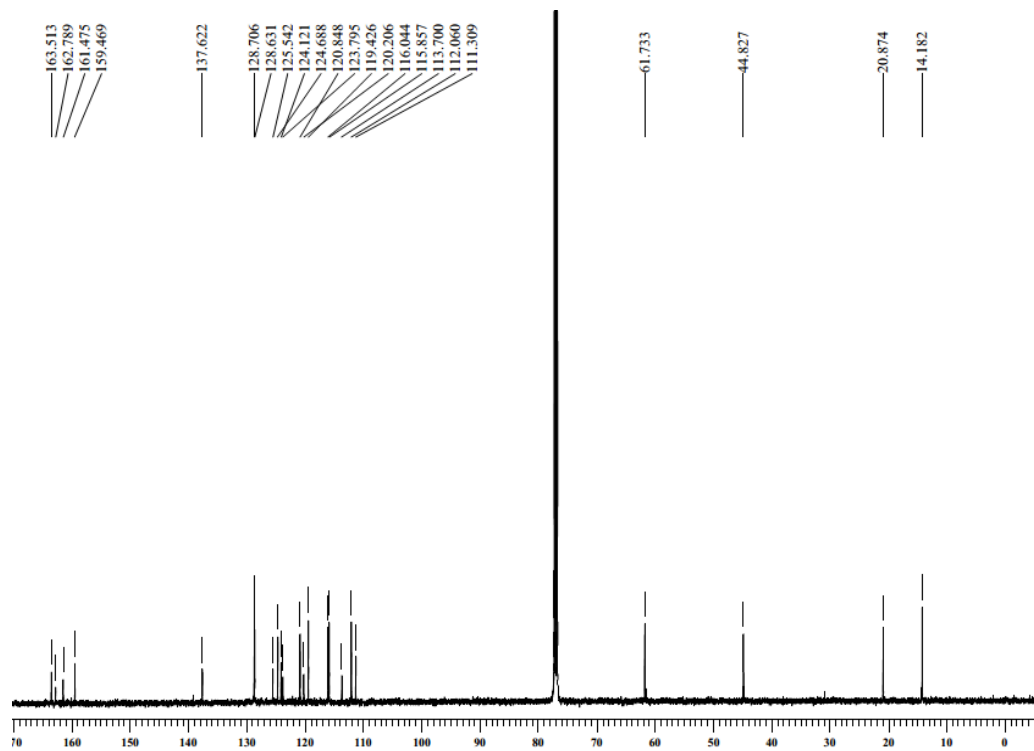
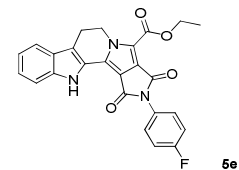
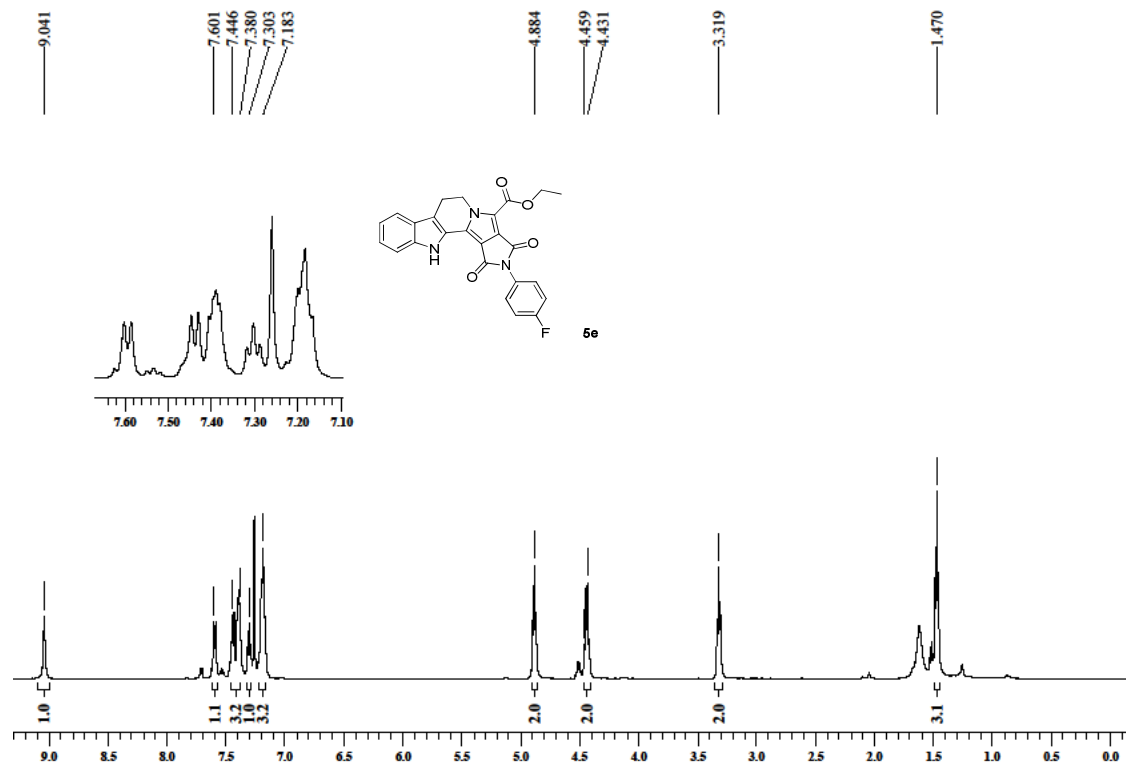
$^1\text{H}$  NMR Spectrum for **5b** ( $\text{CDCl}_3$ , 500 MHz)



$^{13}\text{C}$  NMR Spectrum for **5b** ( $\text{CDCl}_3$ , 125 MHz)

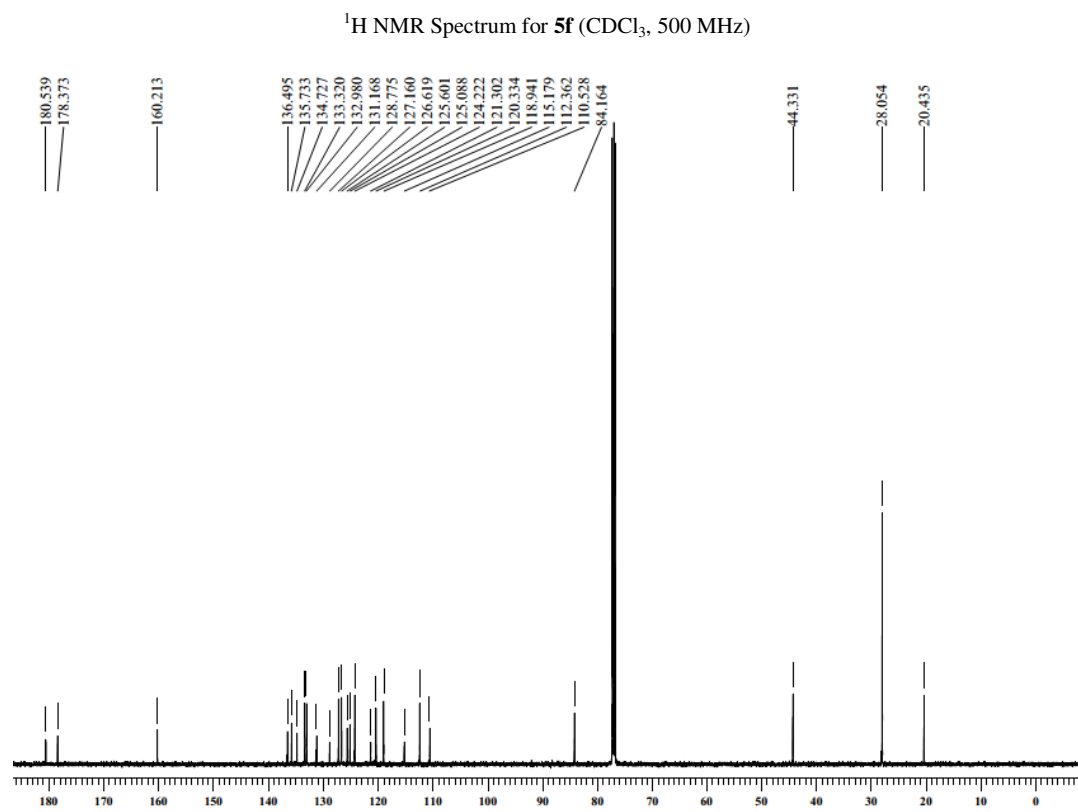
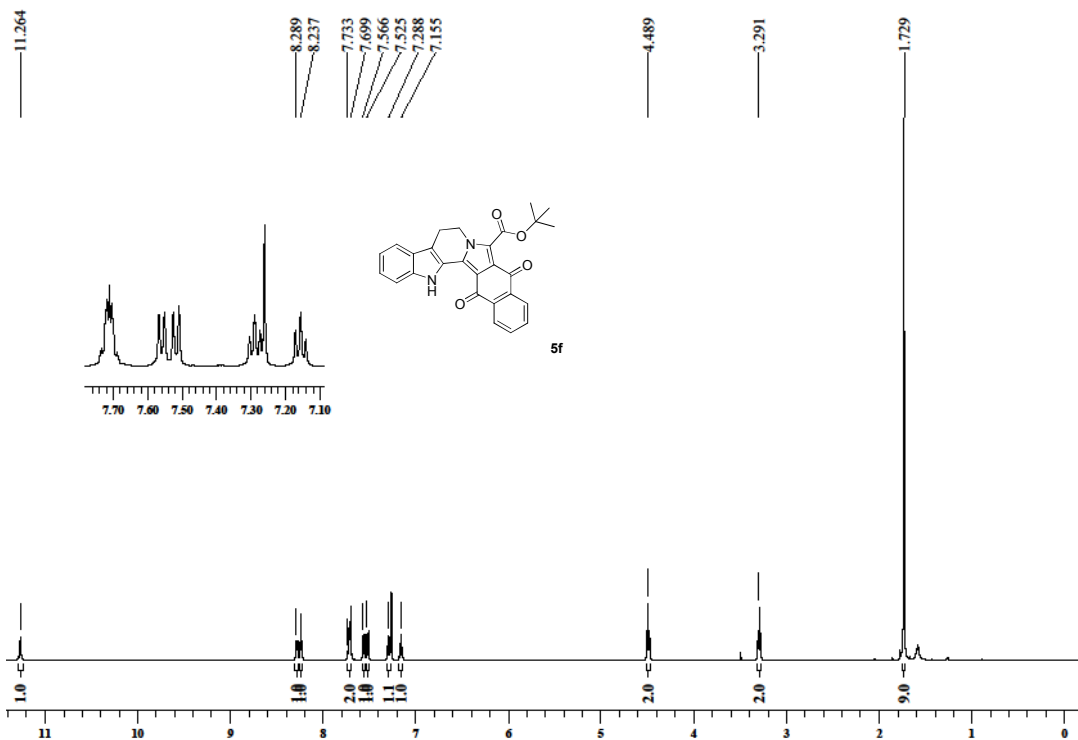


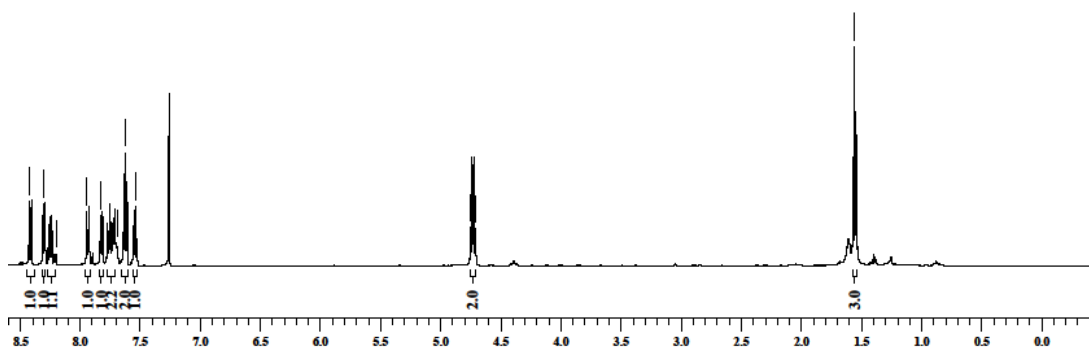
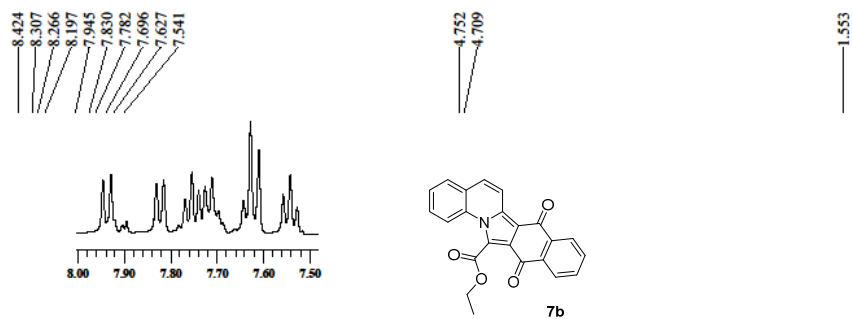




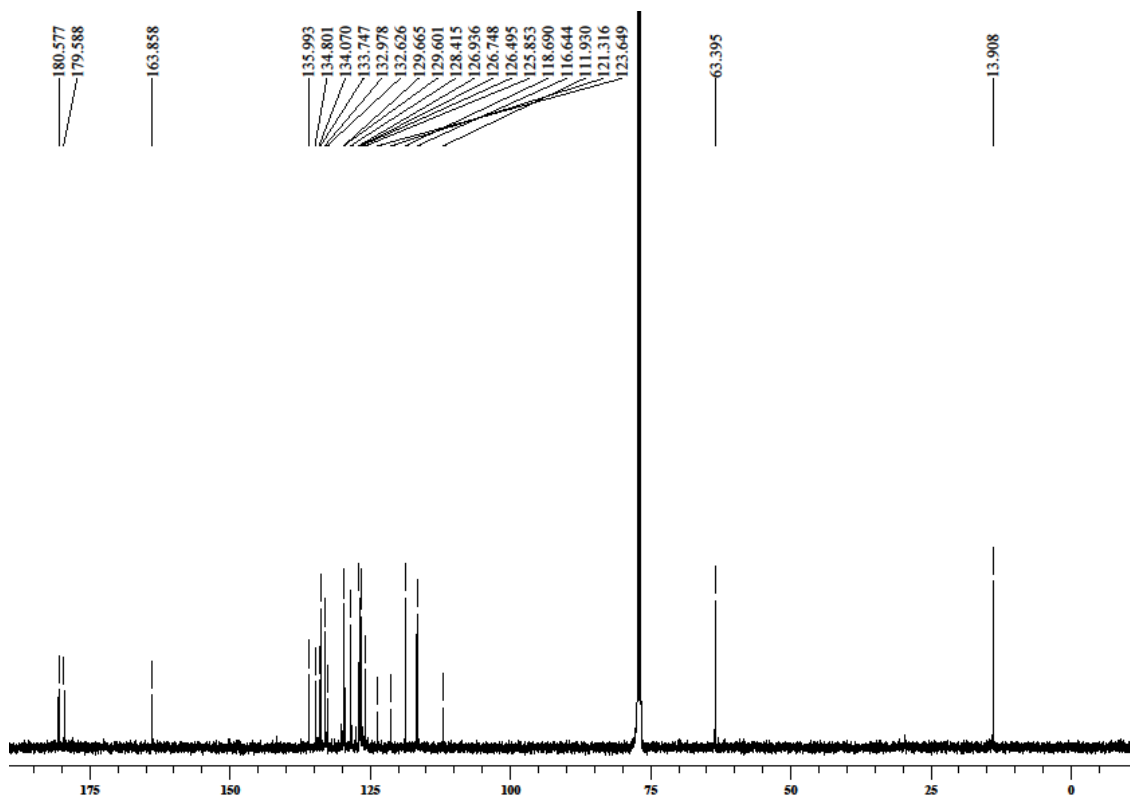
**<sup>13</sup>C NMR Spectrum for 5e (CDCl<sub>3</sub>, 125 MHz)**







$^1\text{H}$  NMR Spectrum for **7d** ( $\text{CDCl}_3$ , 500 Hz)



$^{13}\text{C}$  NMR Spectrum for **7d** ( $\text{CDCl}_3$ , 125 MHz)