

# Supplementary Materials

## Deprotometalation-iodolysis and direct iodination of 1-arylated 7-azaindoles: Reactivity studies and molecule properties

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Technology, Faculty of Public Health, Lebanese University, 1300 Tripoli, Lebanon

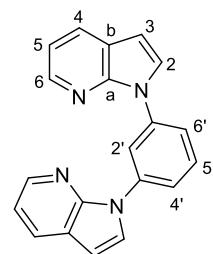
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Belarus

bentabedg@gmail.com (G. Bentabed-Ababsa); ziad.fajloun@ul.edu.lb (Z. Fajloun);

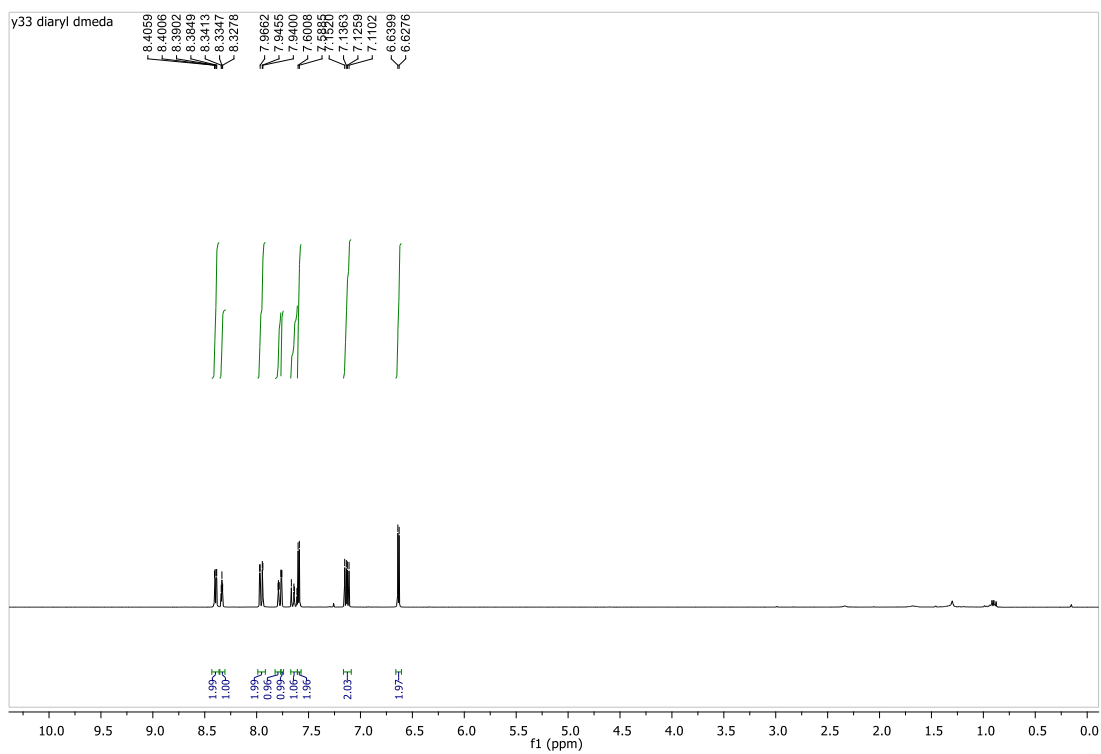
hys@tut.by (Y. S. Halauko); florence.mongin@univ-rennes1.fr (F. Mongin)

NMR data of compounds <b>2k</b> , <b>2k'</b> , <b>3a</b> , <b>3a'</b> , <b>3e-g</b> , <b>3g'</b> , <b>3k</b> , <b>3k'</b> , <b>3k''</b> , <b>4b-f</b> , <b>4h</b> , <b>4i</b> , <b>5e</b> , <b>5i</b> and <b>6g'</b>	p. SM2
Calculated values of the Gibbs energies $\Delta G_{\text{acid}}$ for deprotonation	p. SM33
Cartesian coordinates of molecular geometry for the most stable rotamer form optimized at the B3LYP/6-31G(d) level of theory	see separate file in the .xyz format

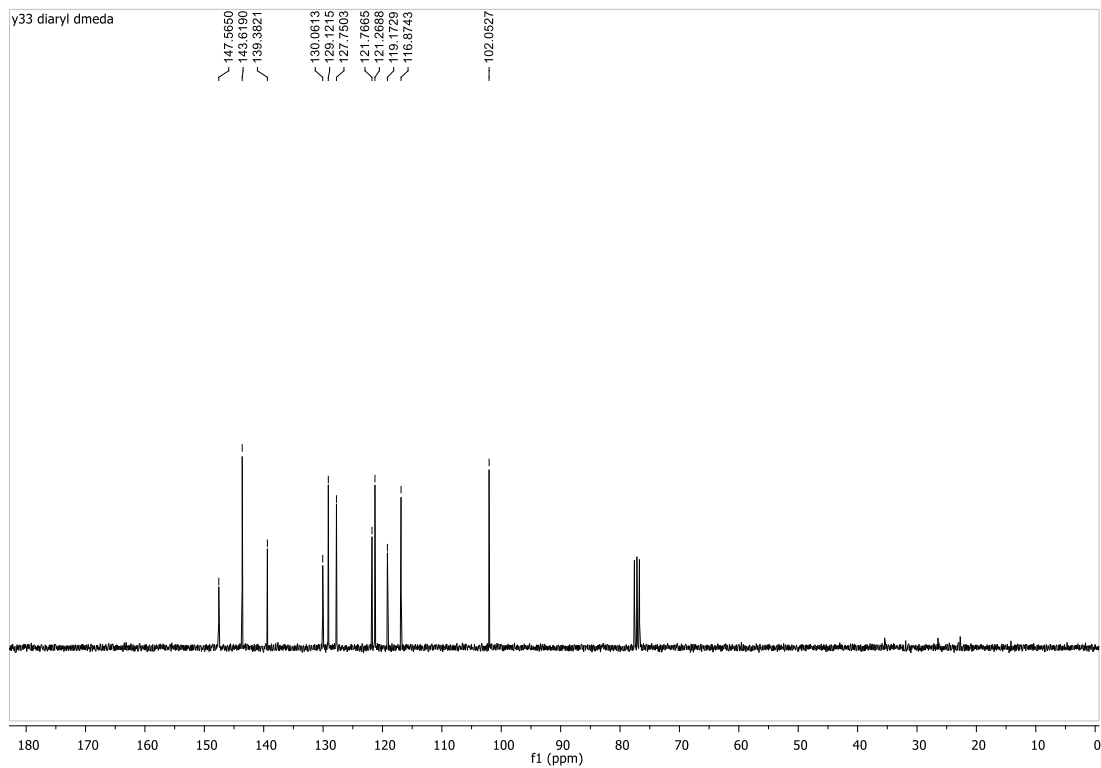


# **1,1'-(1,3-Phenylene)bis(1*H*-pyrrolo[2,3-*b*]pyridine) (2k)**

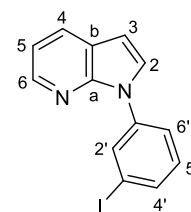
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



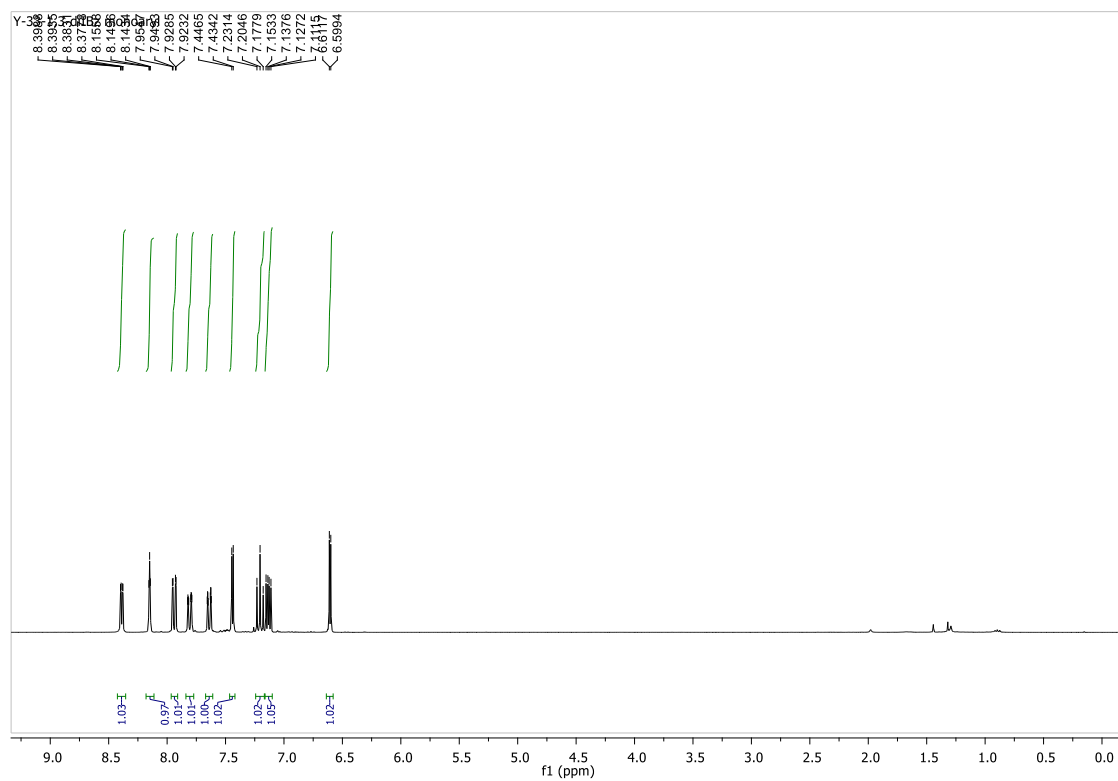
<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)



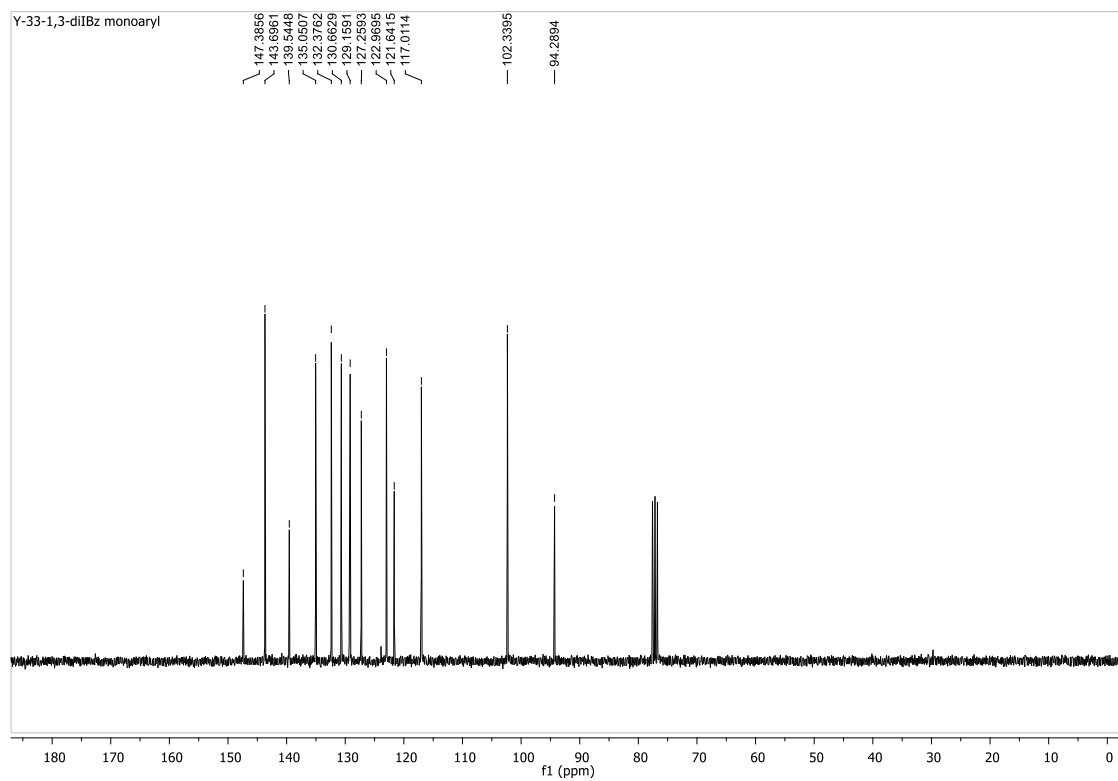
# 1-(3-Iodophenyl)-1*H*-pyrrolo[2,3-*b*]pyridine (2k')



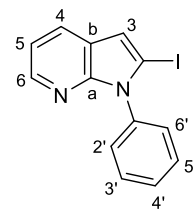
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



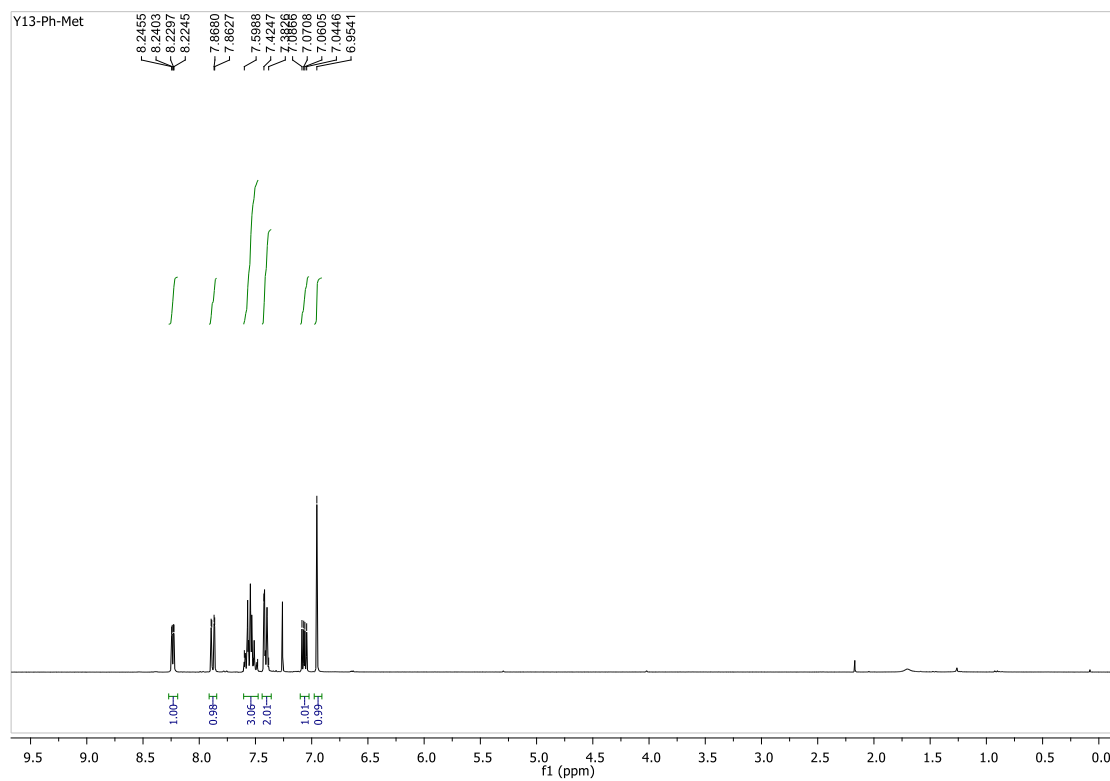
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



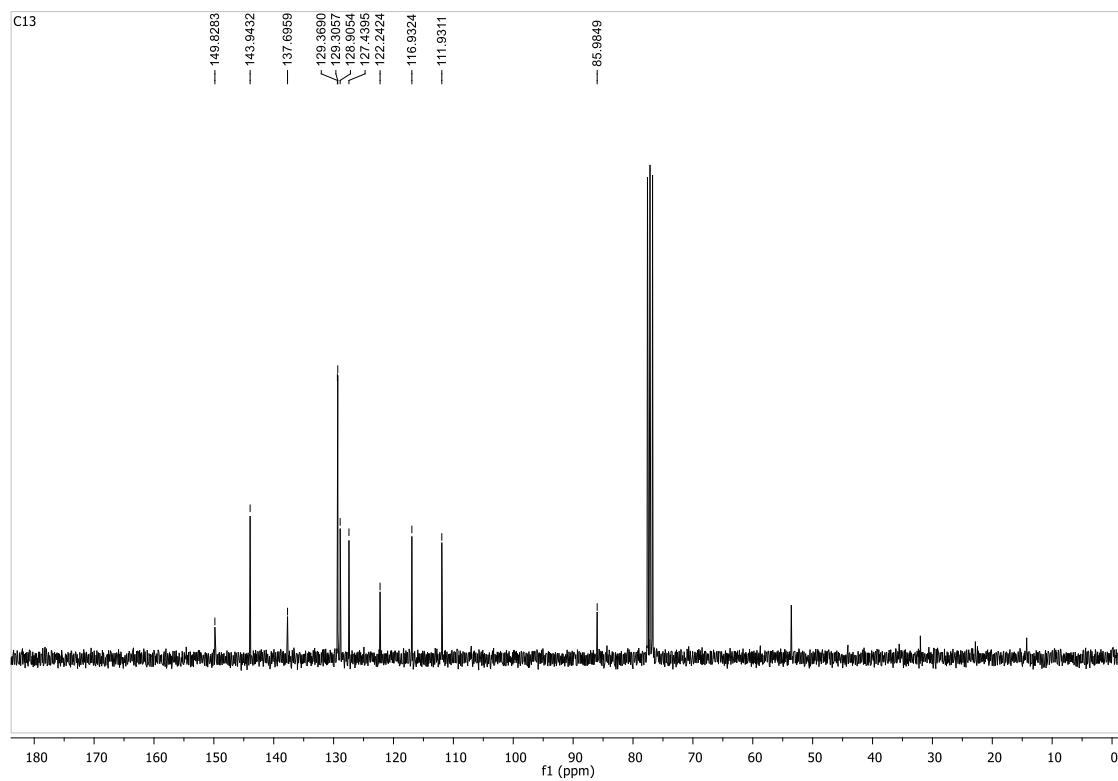
## 2-Iodo-1-phenyl-1*H*-pyrrolo[2,3-*b*]pyridine (3a)



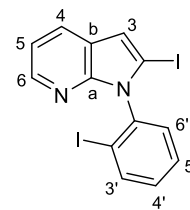
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



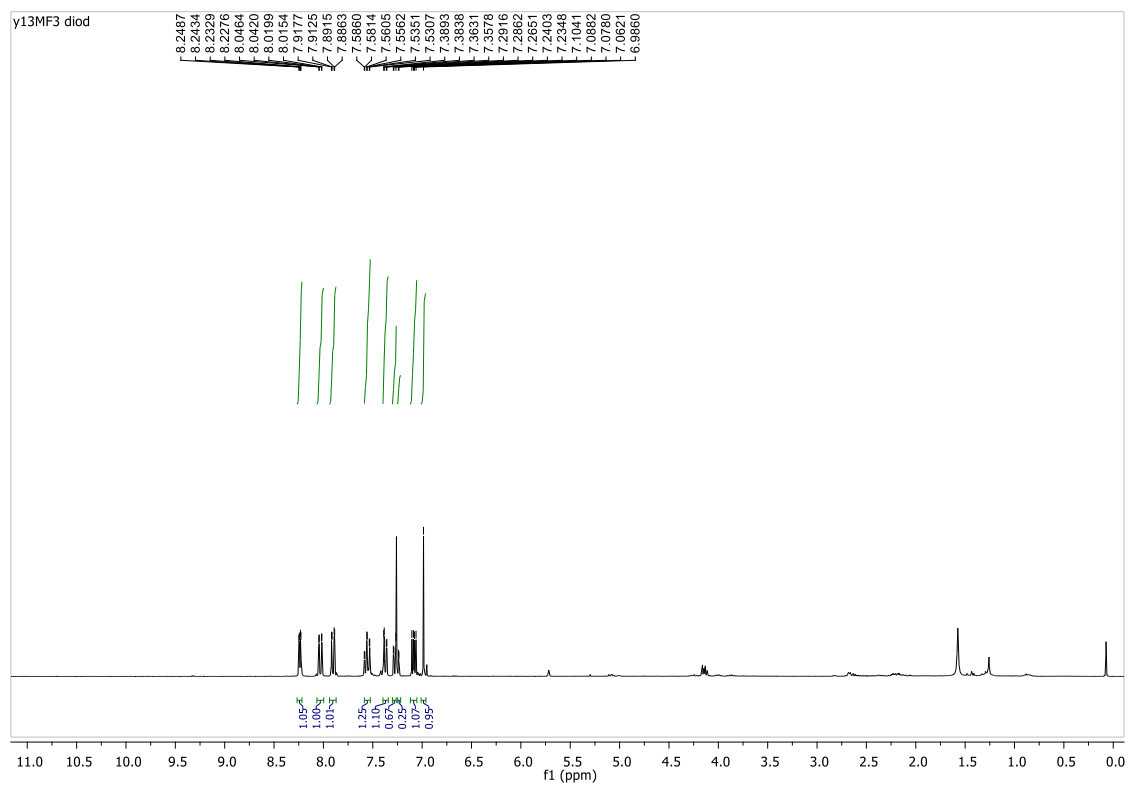
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



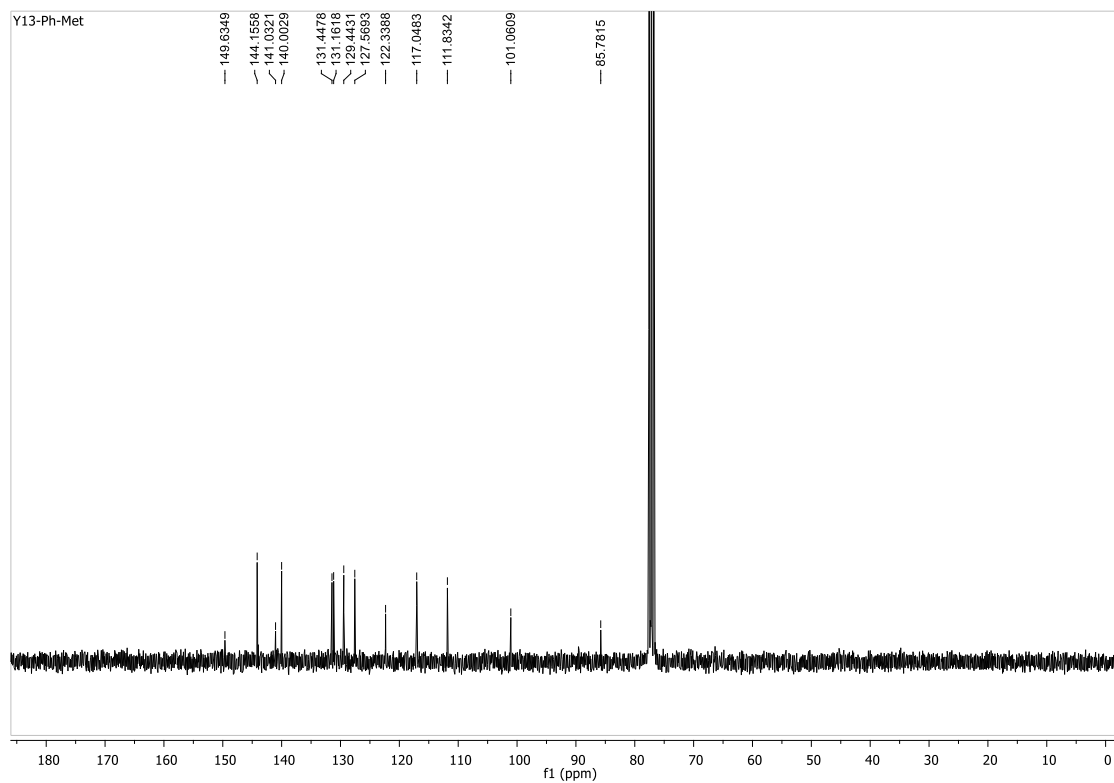
## 2-Iodo-1-(2-iodophenyl)-1*H*-pyrrolo[2,3-*b*]pyridine (3a')



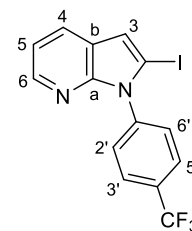
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



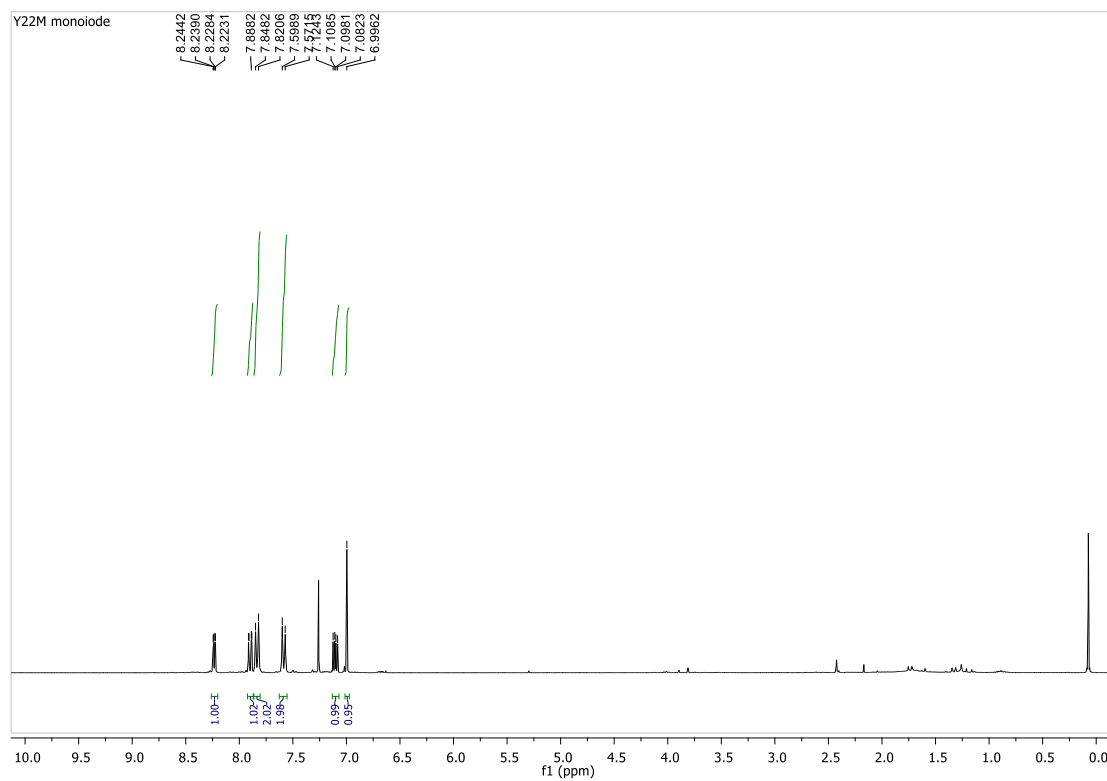
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



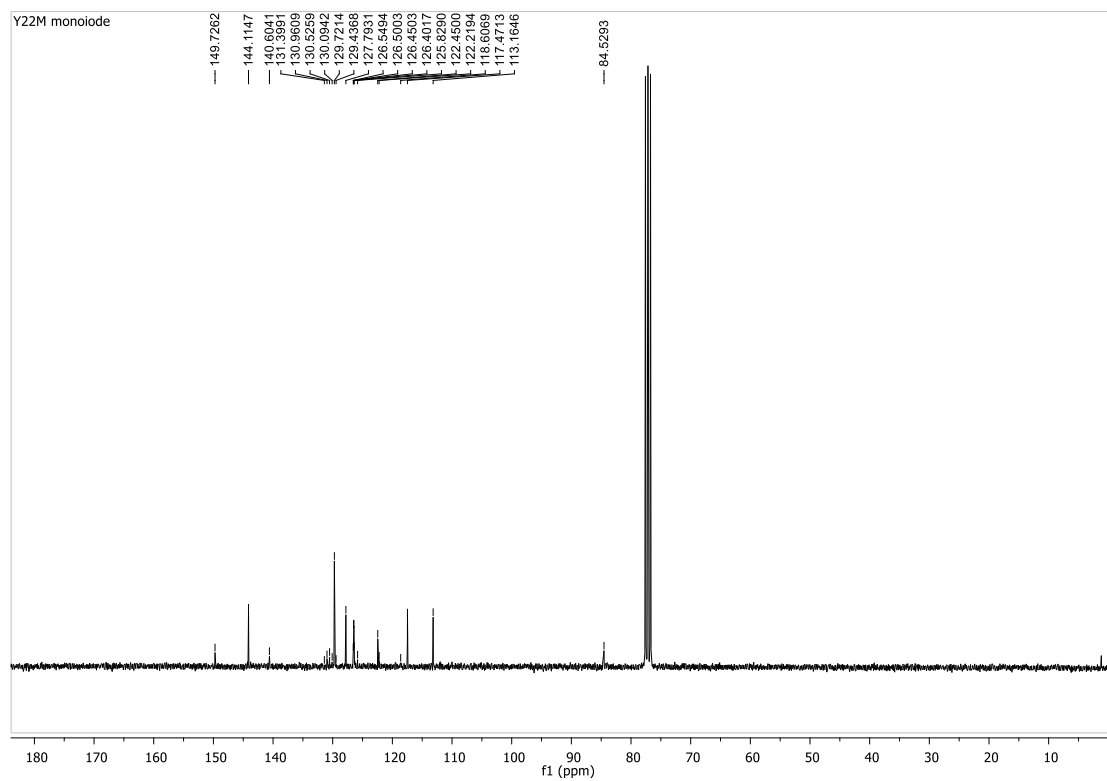
## 2-Iodo-1-(4-(trifluoromethyl)phenyl)-1*H*-pyrrolo[2,3-*b*]pyridine (3e)



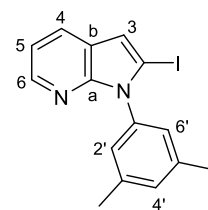
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



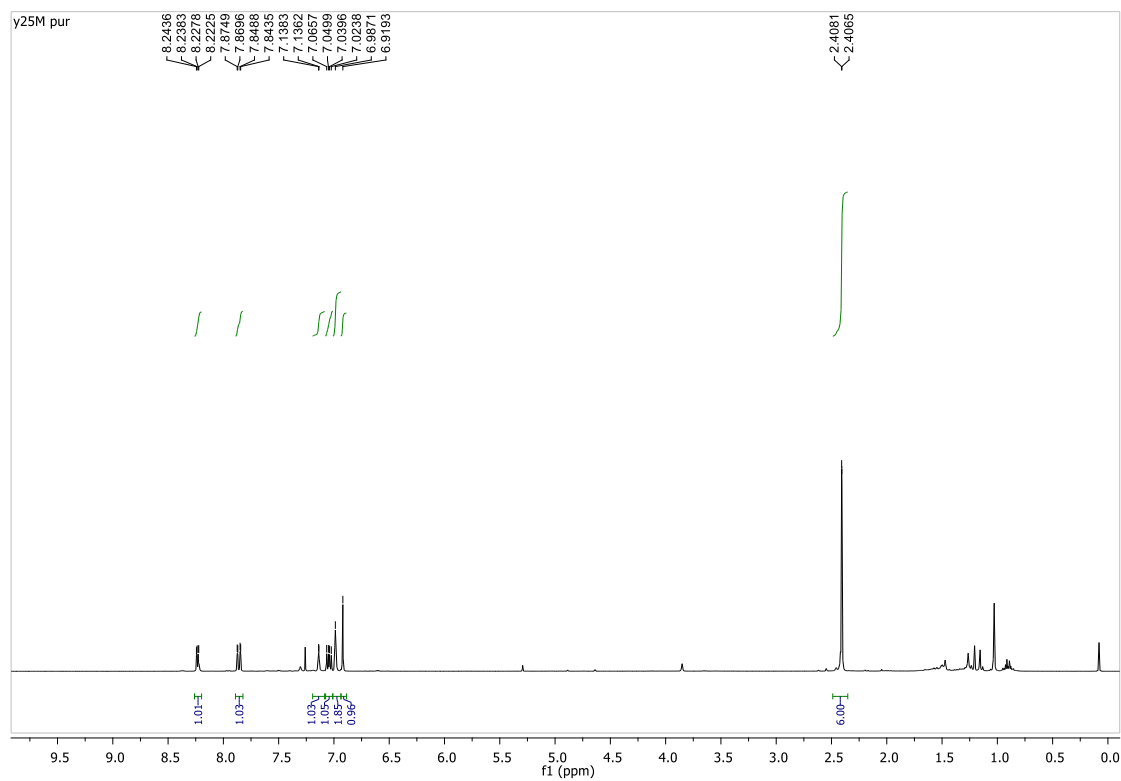
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



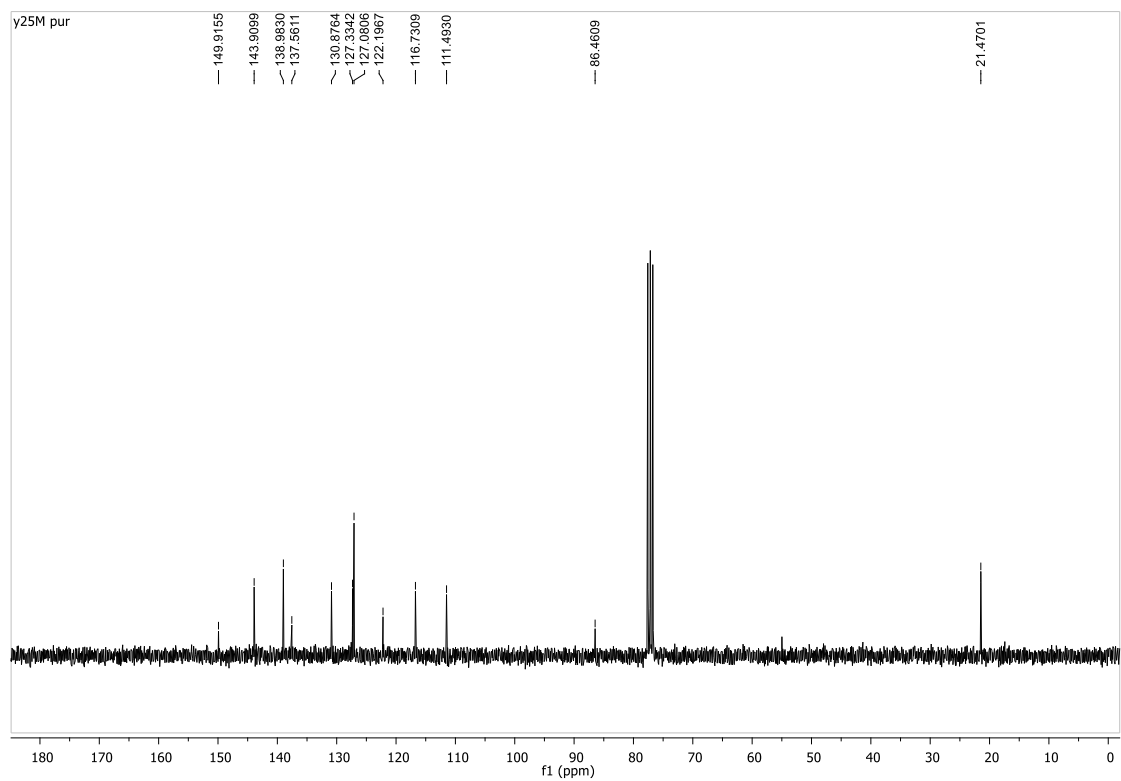
# 1-(3,5-Dimethylphenyl)-2-iodo-1*H*-pyrrolo[2,3-*b*]pyridine (3f)



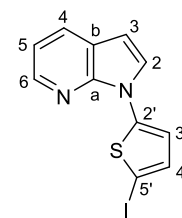
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



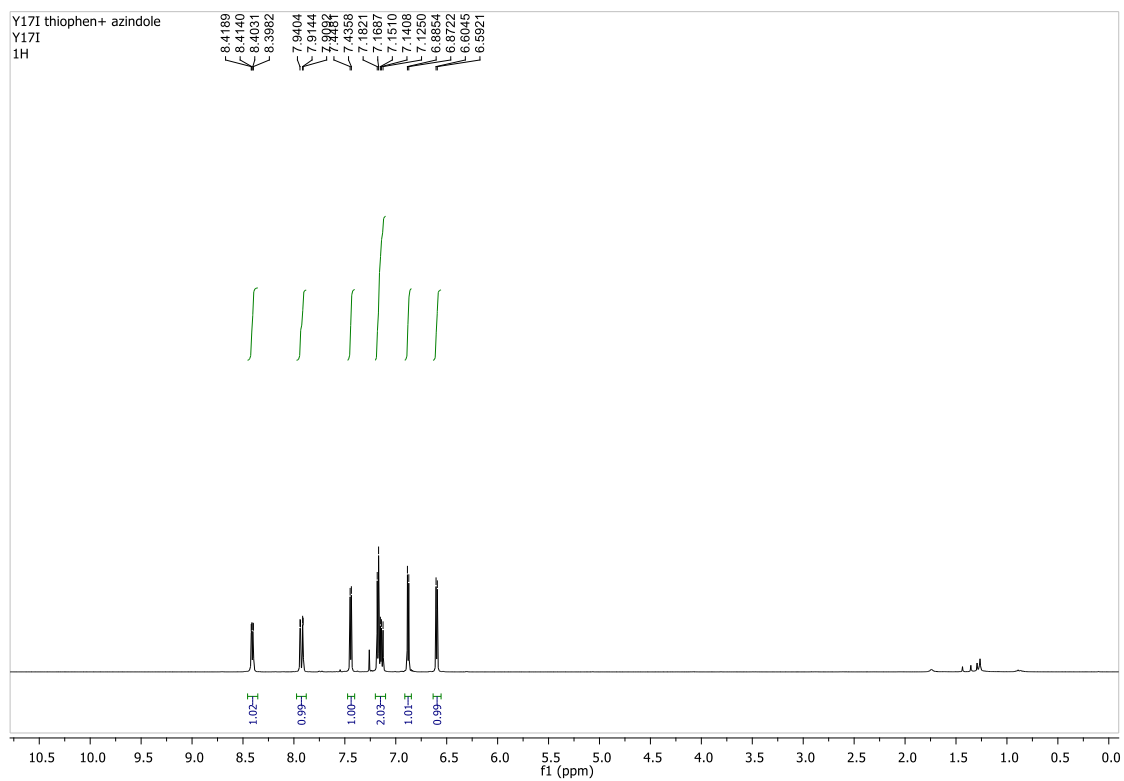
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



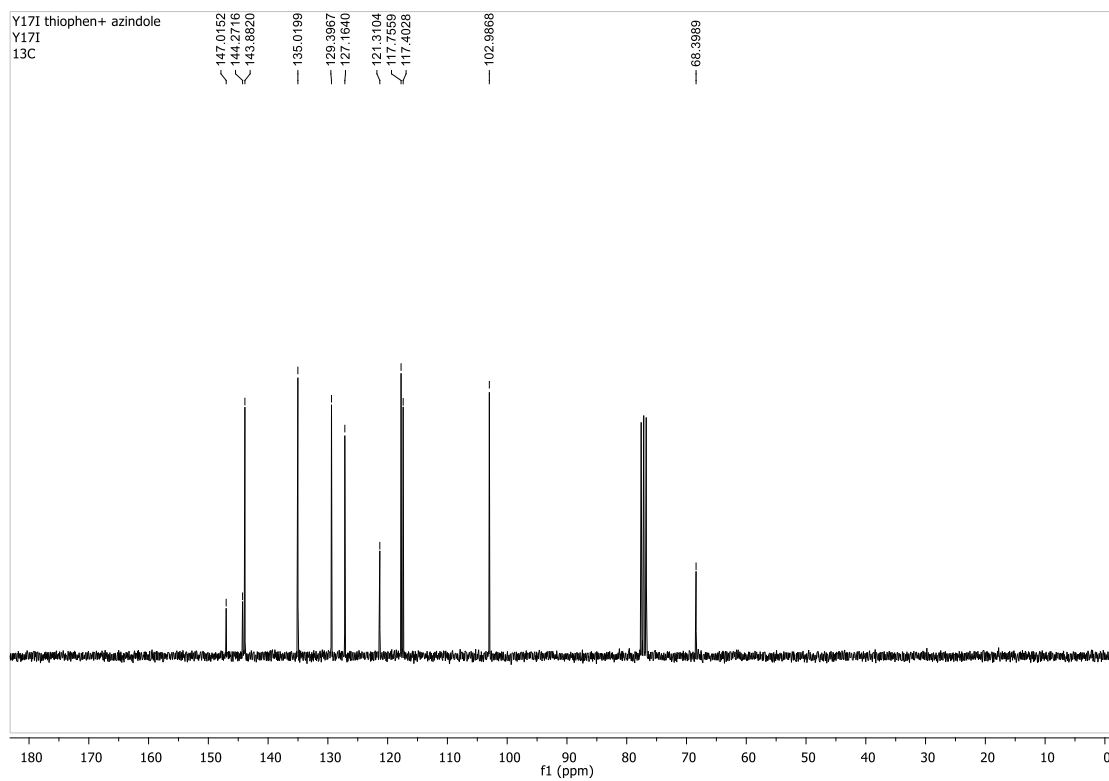
# 1-(5-Iodo-2-thienyl)-1*H*-pyrrolo[2,3-*b*]pyridine (3g)



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )

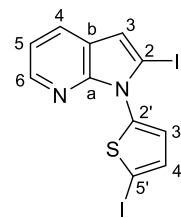


$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )

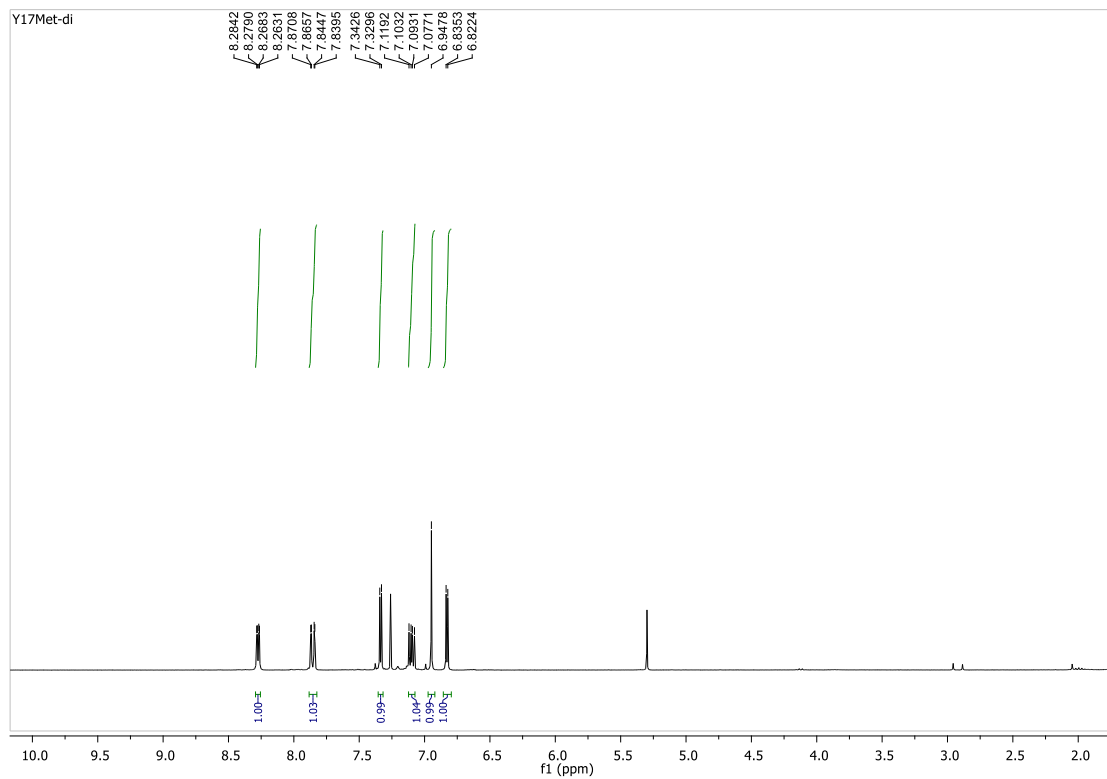




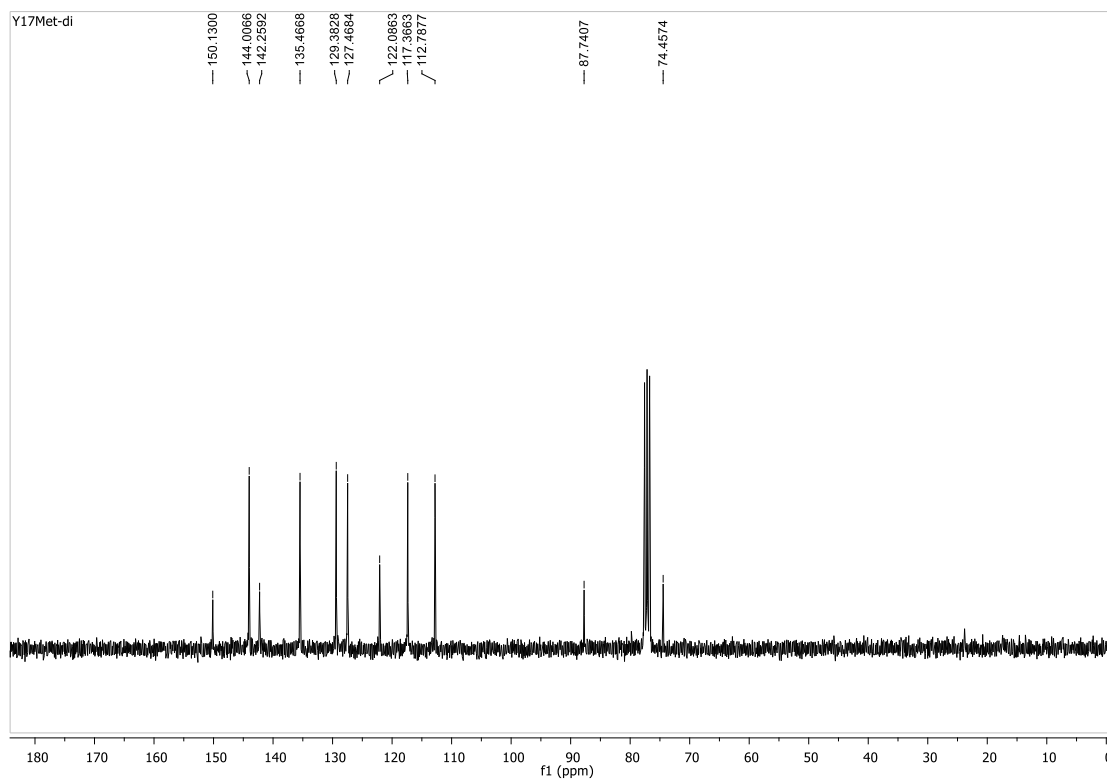
## 2-Iodo-1-(5-iodo-2-thienyl)-1*H*-pyrrolo[2,3-*b*]pyridine (3g')



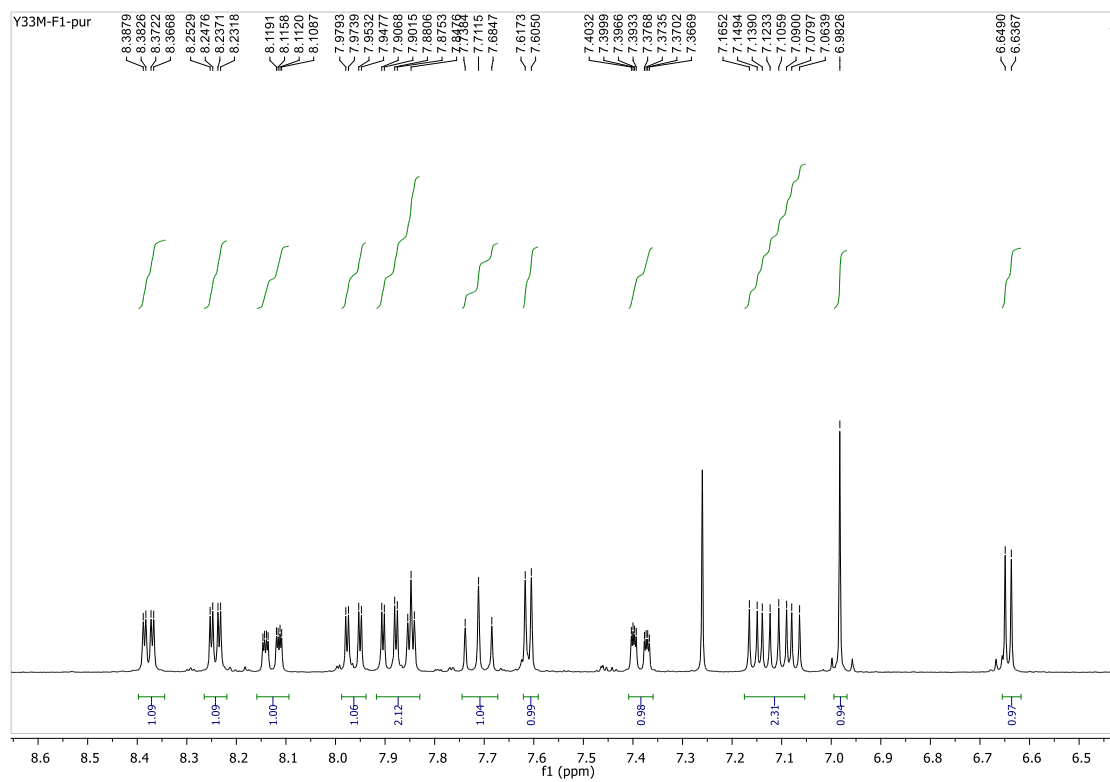
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )

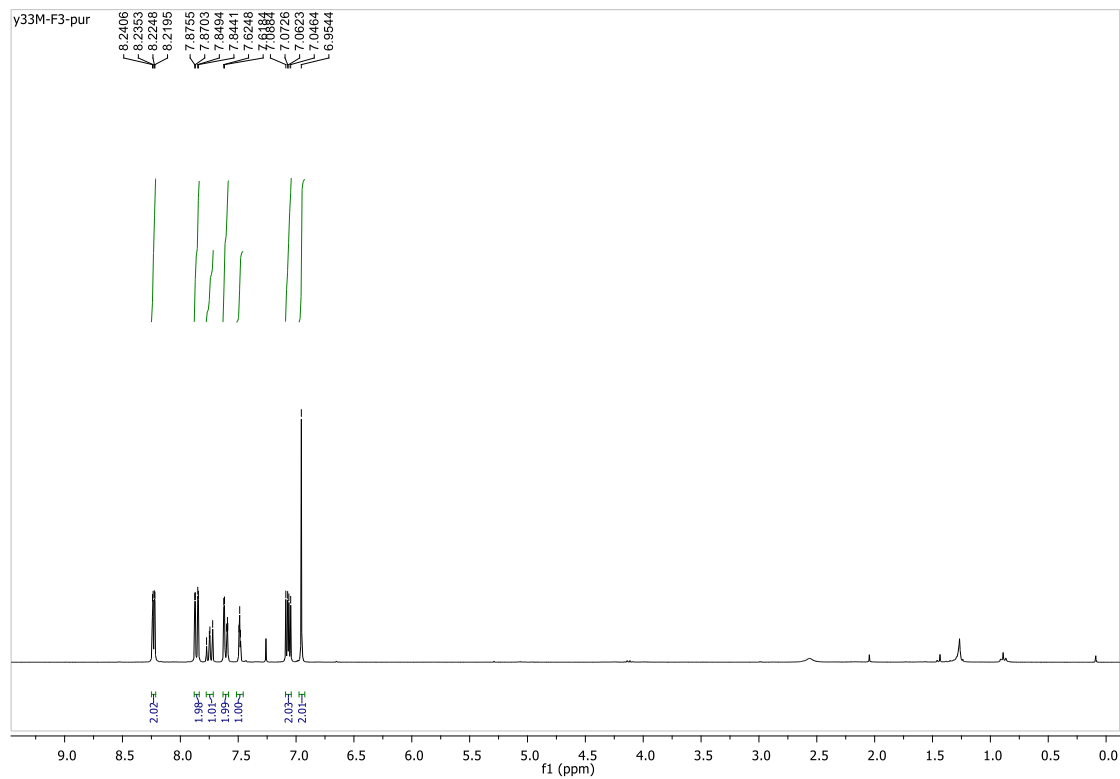
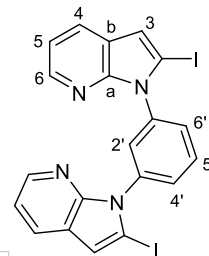


## 2-Iodo-1-(3-(7-azaindoly)phenyl)-7-azaindole (3k)

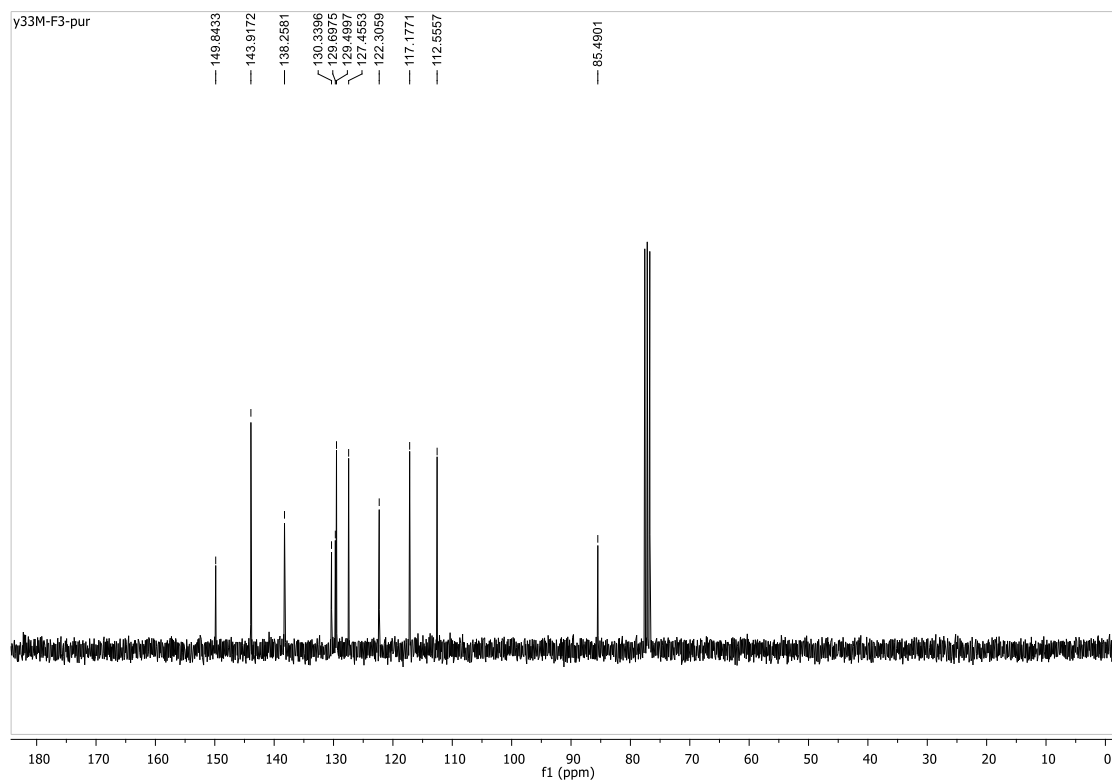


# 1,1'-(1,3-Phenylene)bis(2-iodo-1*H*-pyrrolo[2,3-*b*]pyridine) (3k')

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)

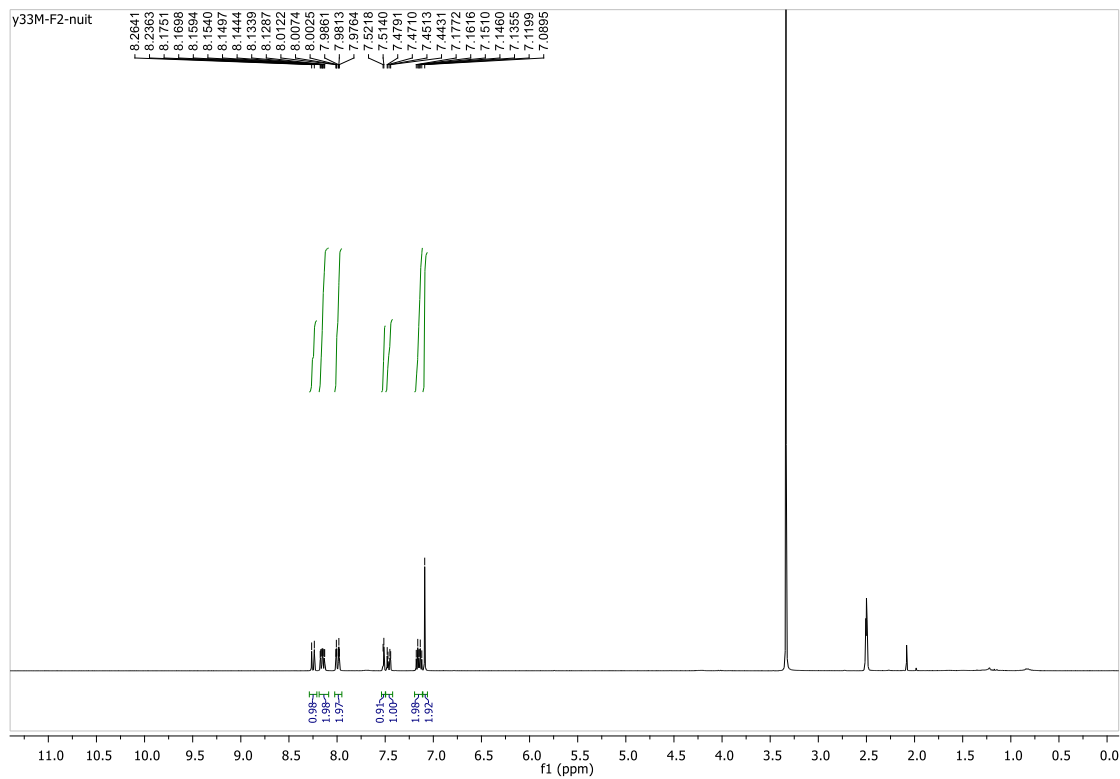


<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

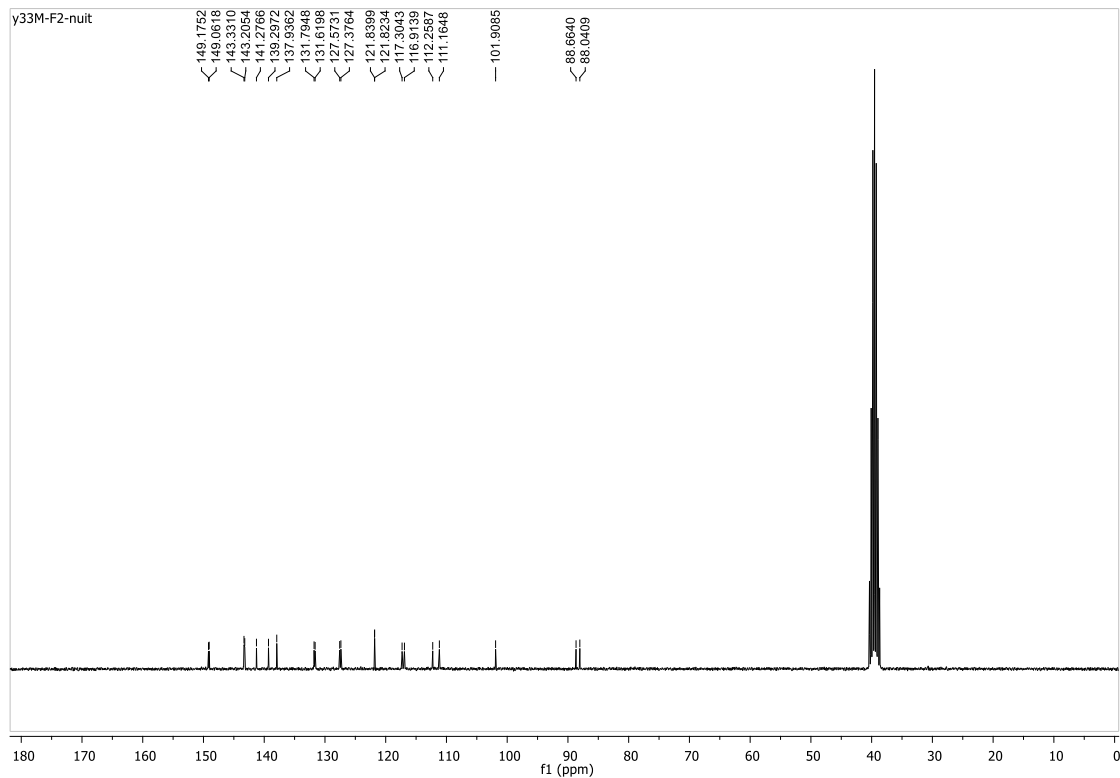


# 1,1'-(1-Iodo-2,4-phenylene)bis(2-iodo-1*H*-pyrrolo[2,3-*b*]pyridine (3k'')

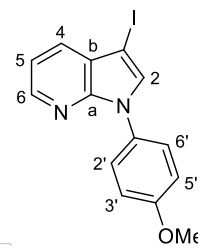
<sup>1</sup>H NMR (300 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)



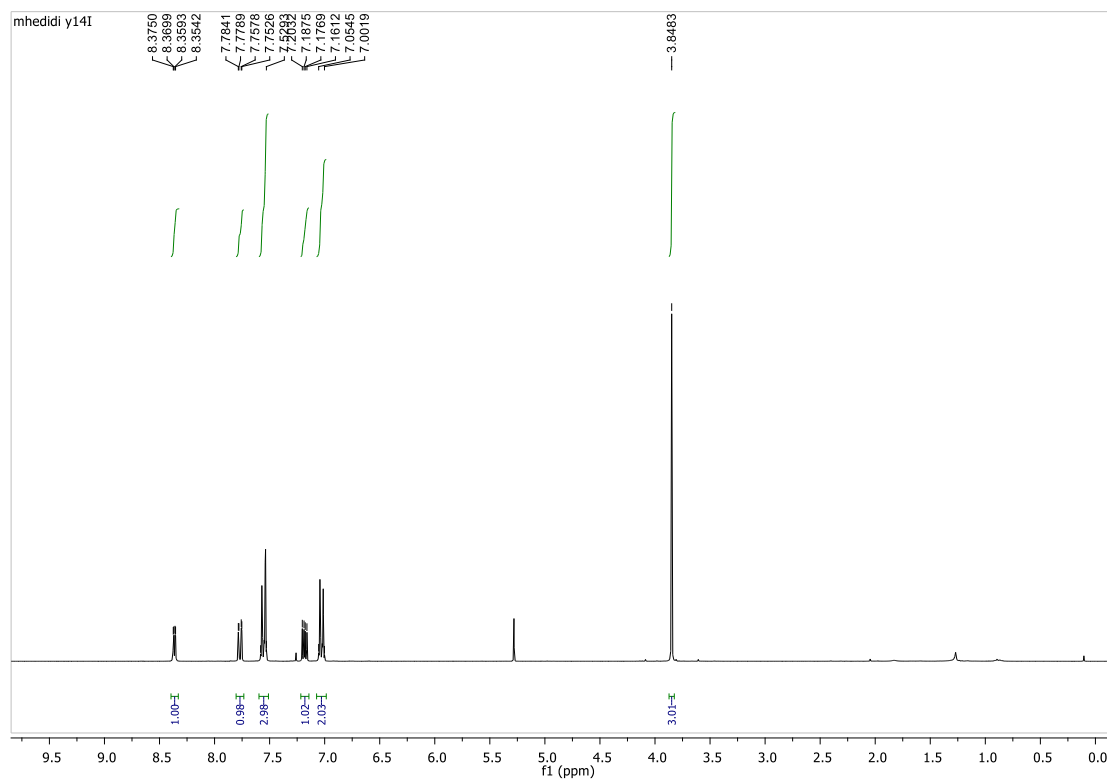
<sup>13</sup>C NMR (75 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)



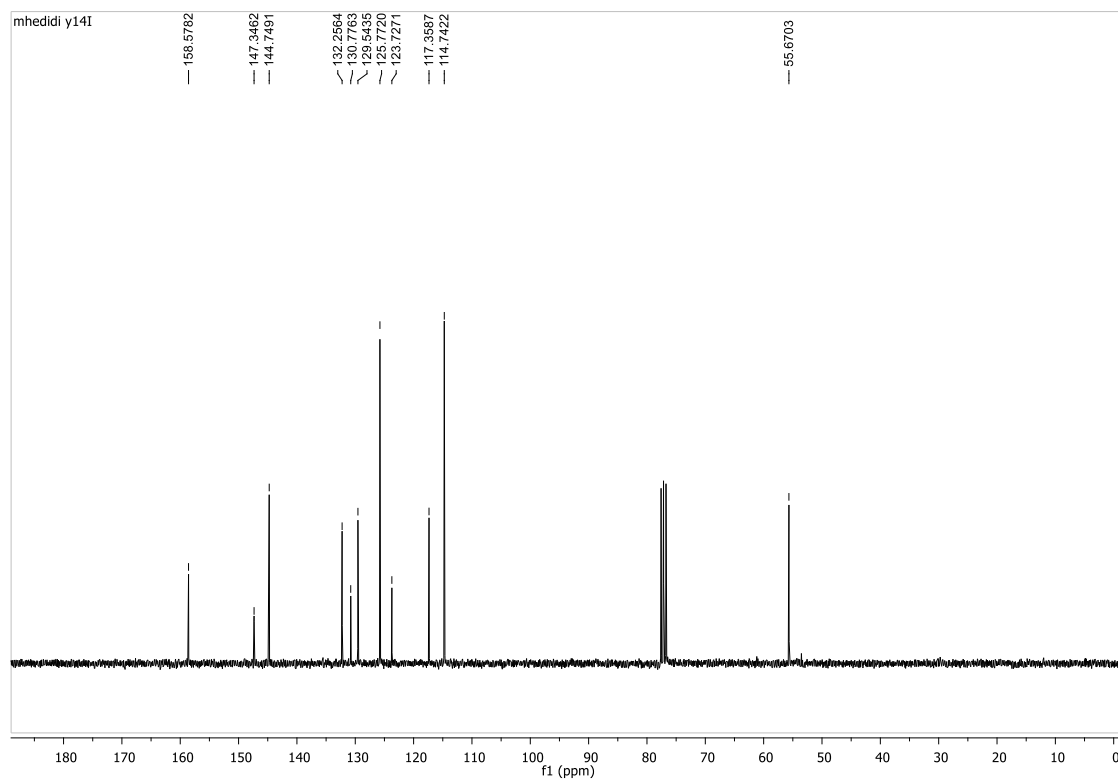
### 3-Iodo-1-(4-methoxyphenyl)-1*H*-pyrrolo[2,3-*b*]pyridine (4b)



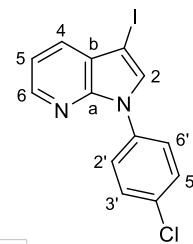
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



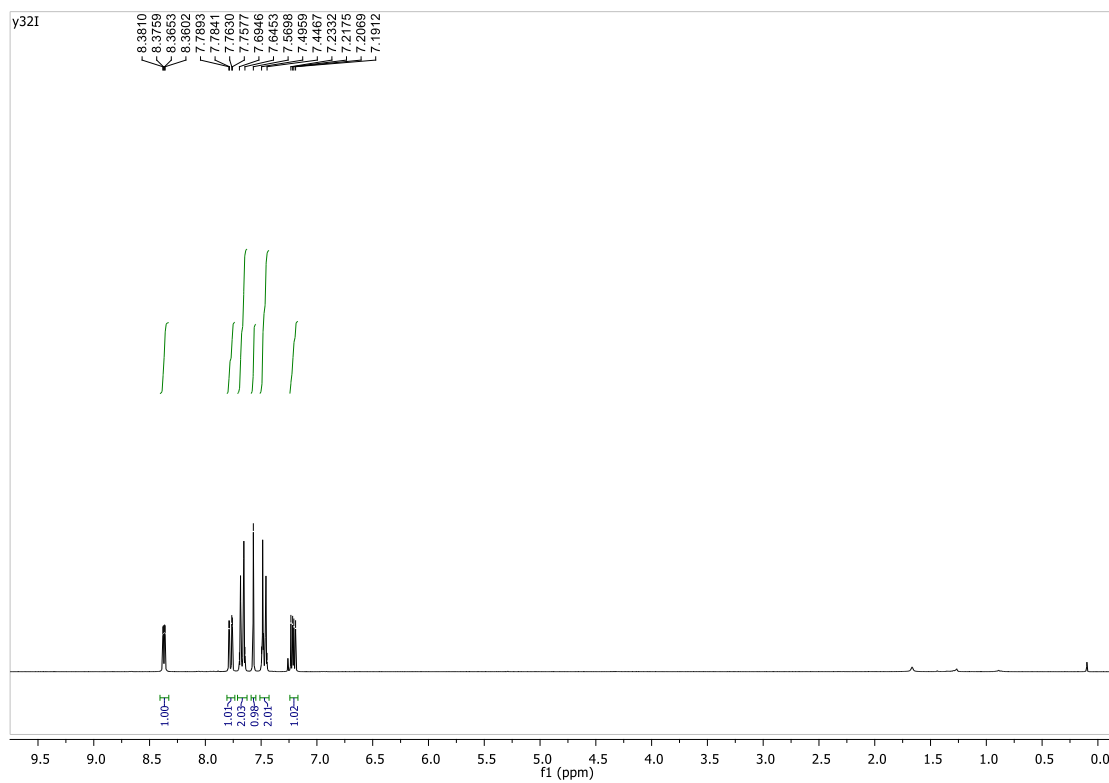
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



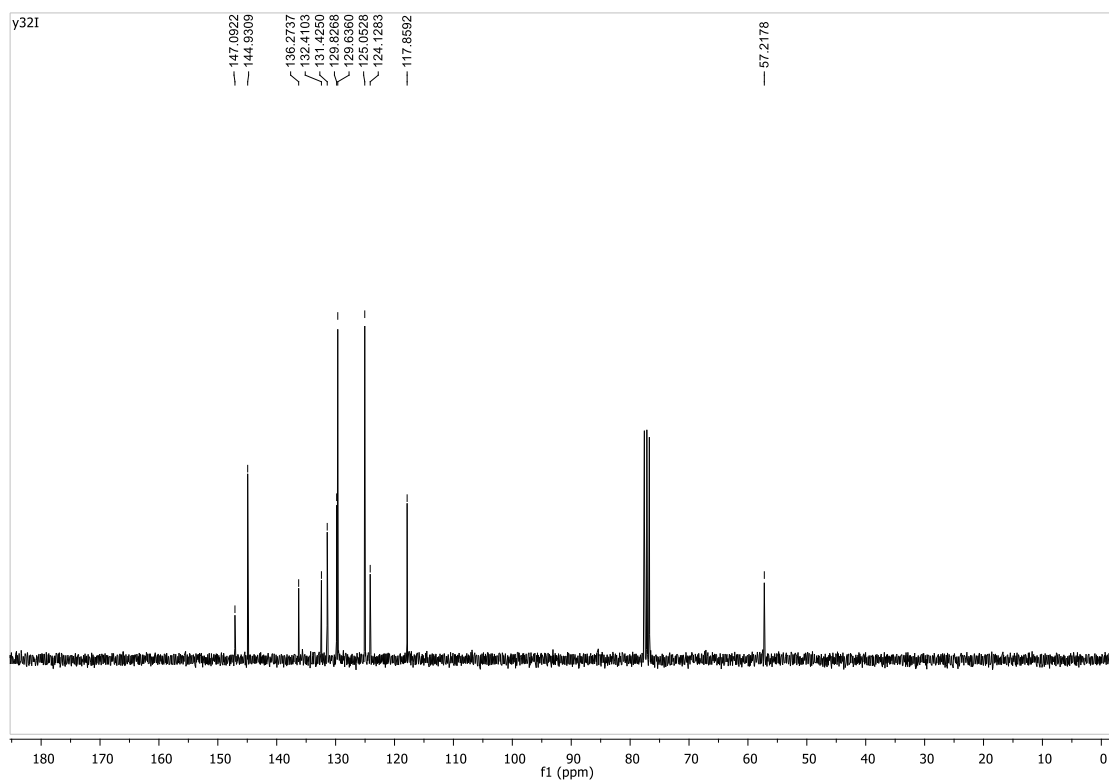
# 1-(4-Chlorophenyl)-3-iodo-1*H*-pyrrolo[2,3-*b*]pyridine (4c)



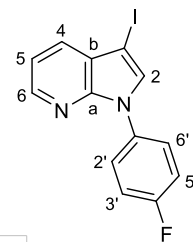
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



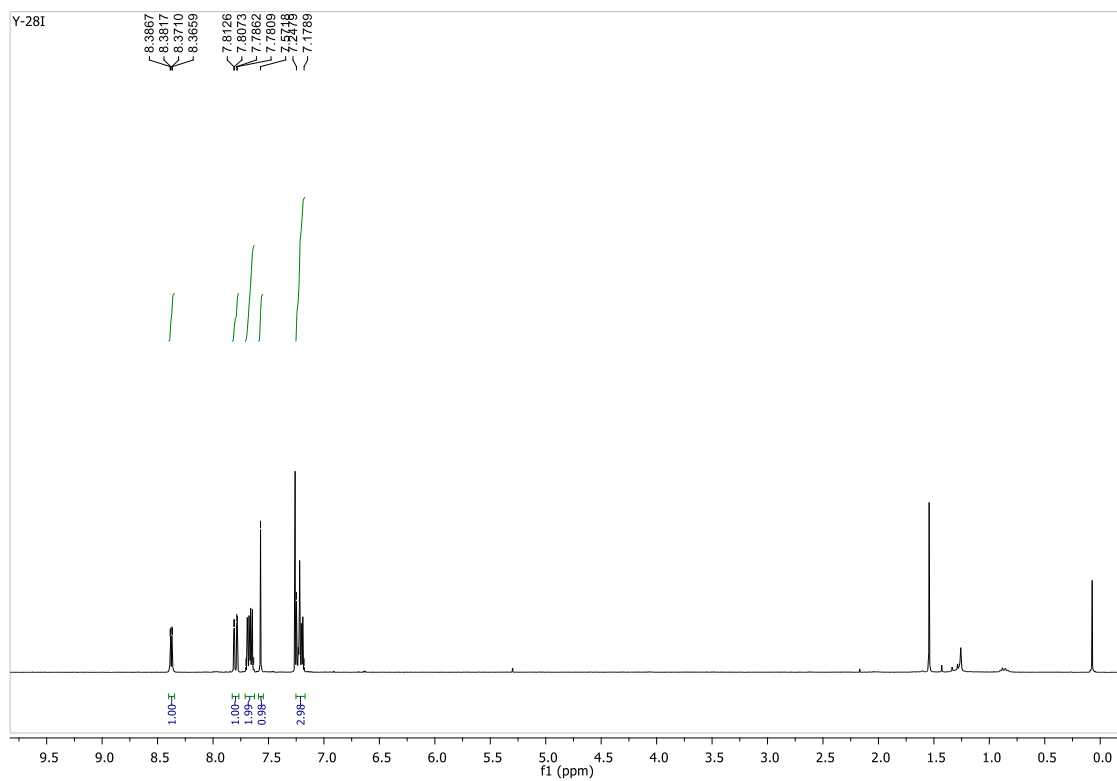
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



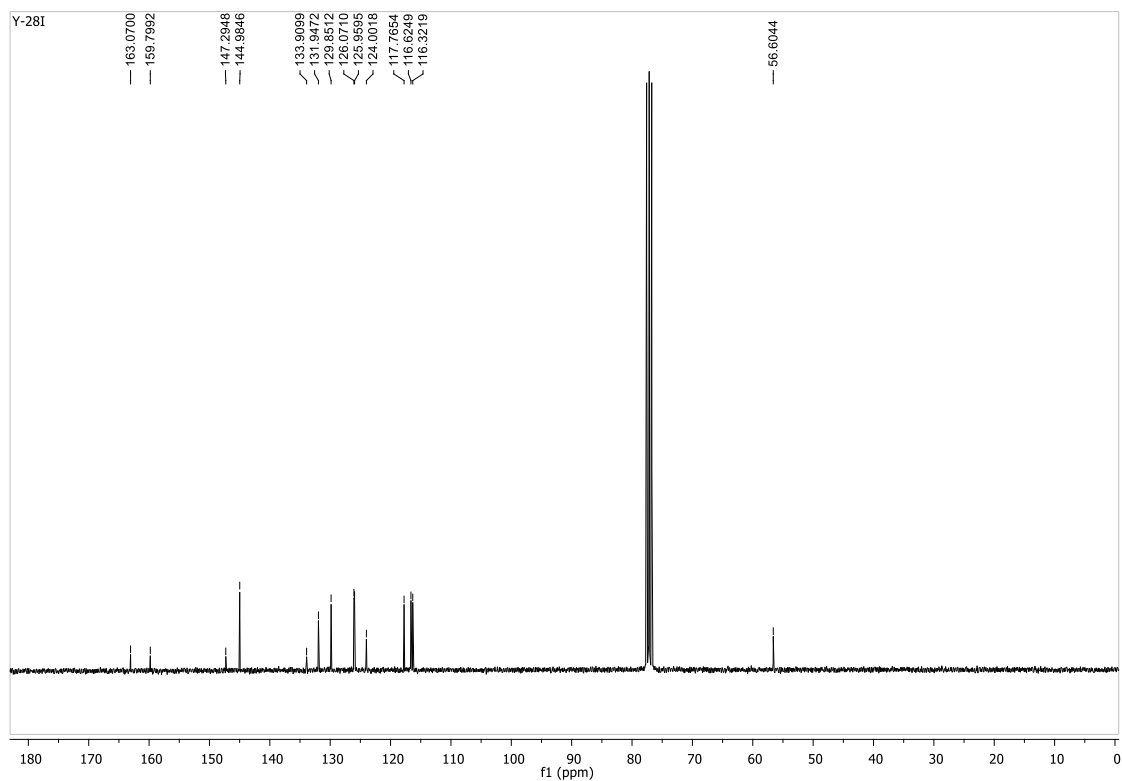
# 1-(4-Fluorophenyl)-3-iodo-1*H*-pyrrolo[2,3-*b*]pyridine (4d)



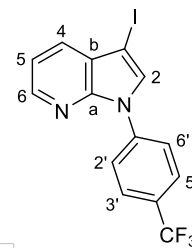
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



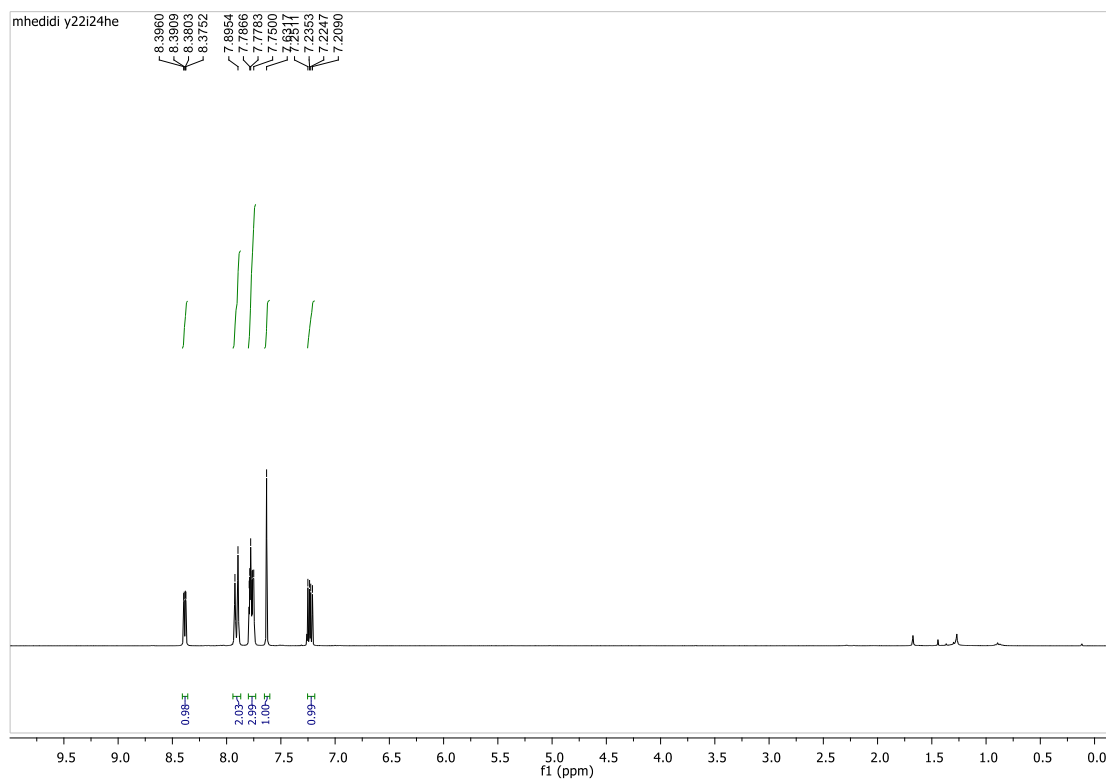
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



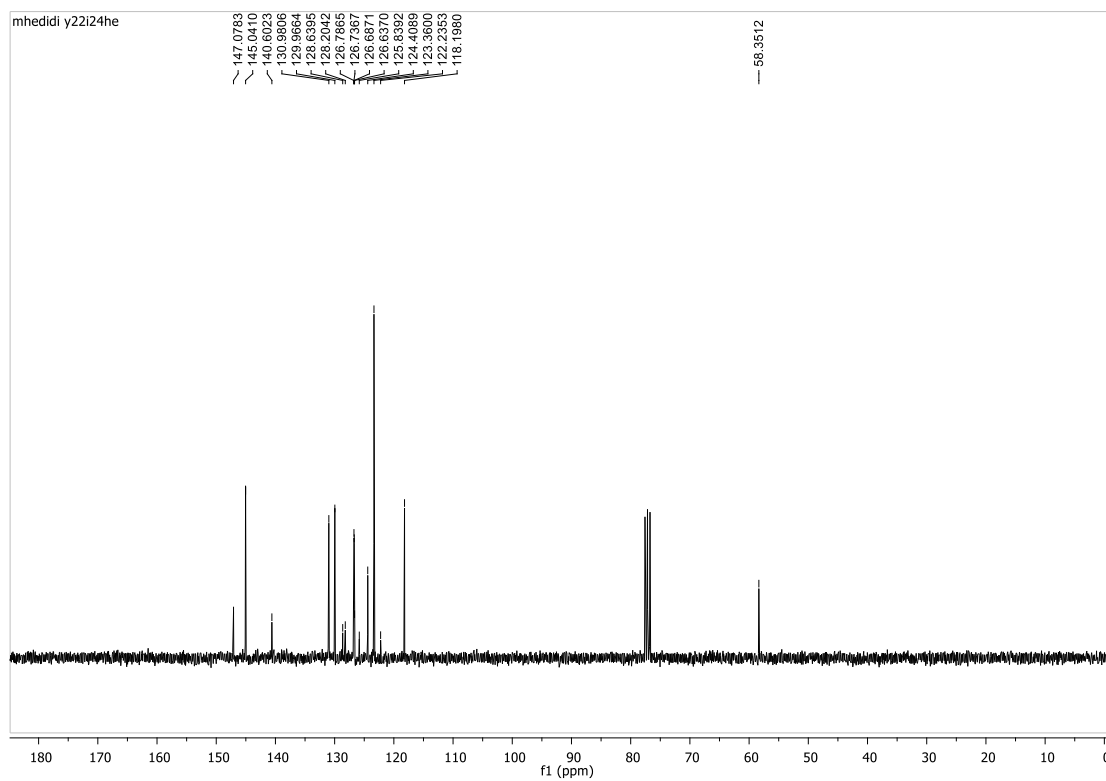
### 3-Iodo-1-(4-(trifluoromethyl)phenyl)-1*H*-pyrrolo[2,3-*b*]pyridine (4e)



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )

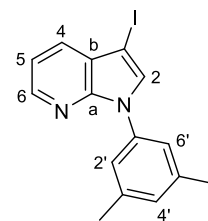


$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )

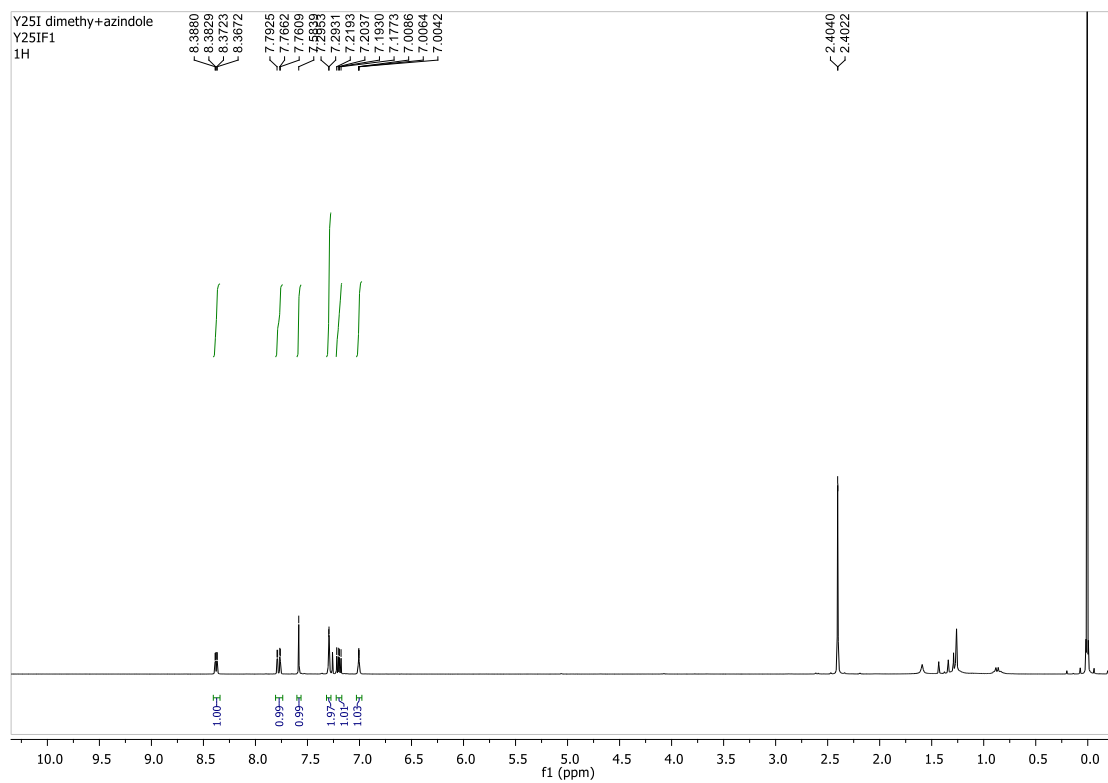




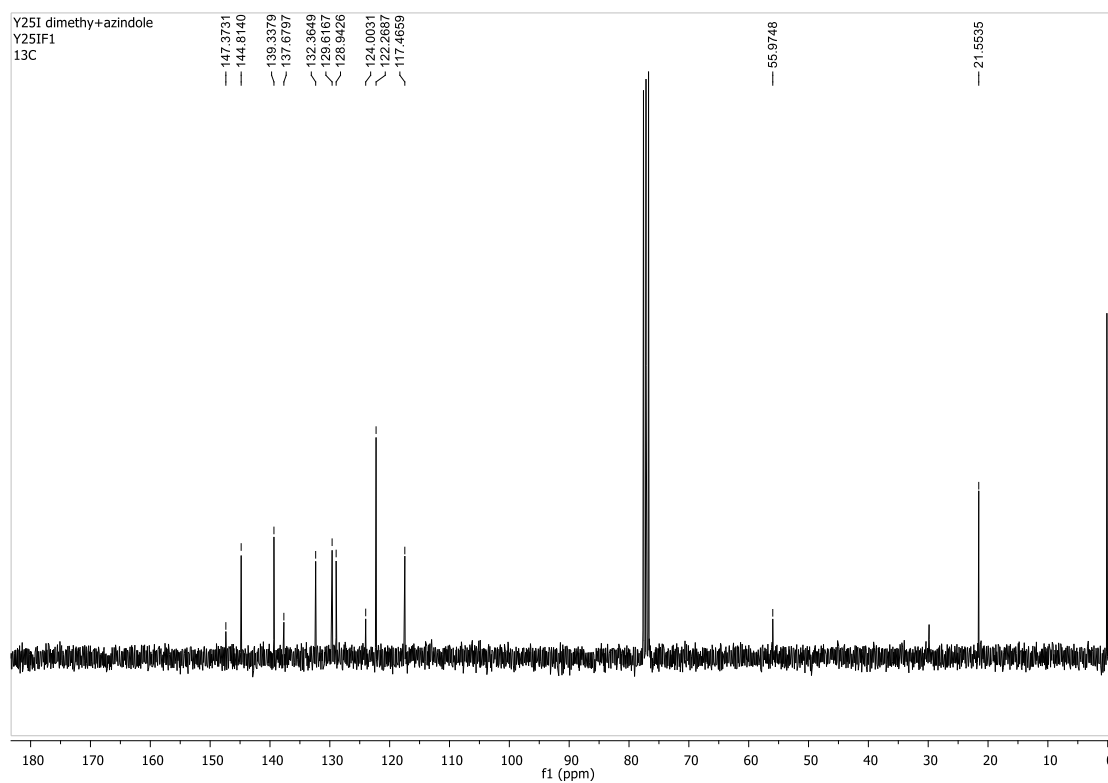
### 3-Iodo-1-(3,5-dimethylphenyl)-1H-pyrrolo[2,3-*b*]pyridine (4f)



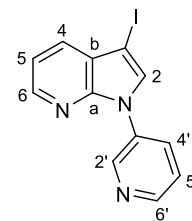
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



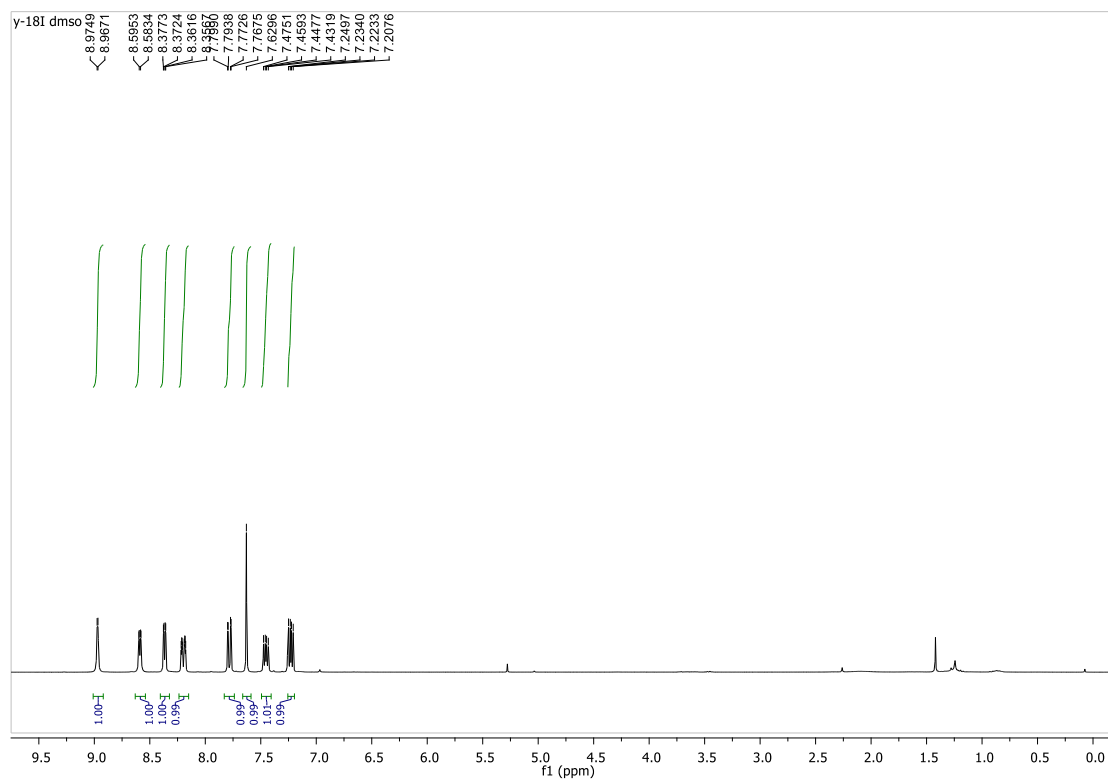
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



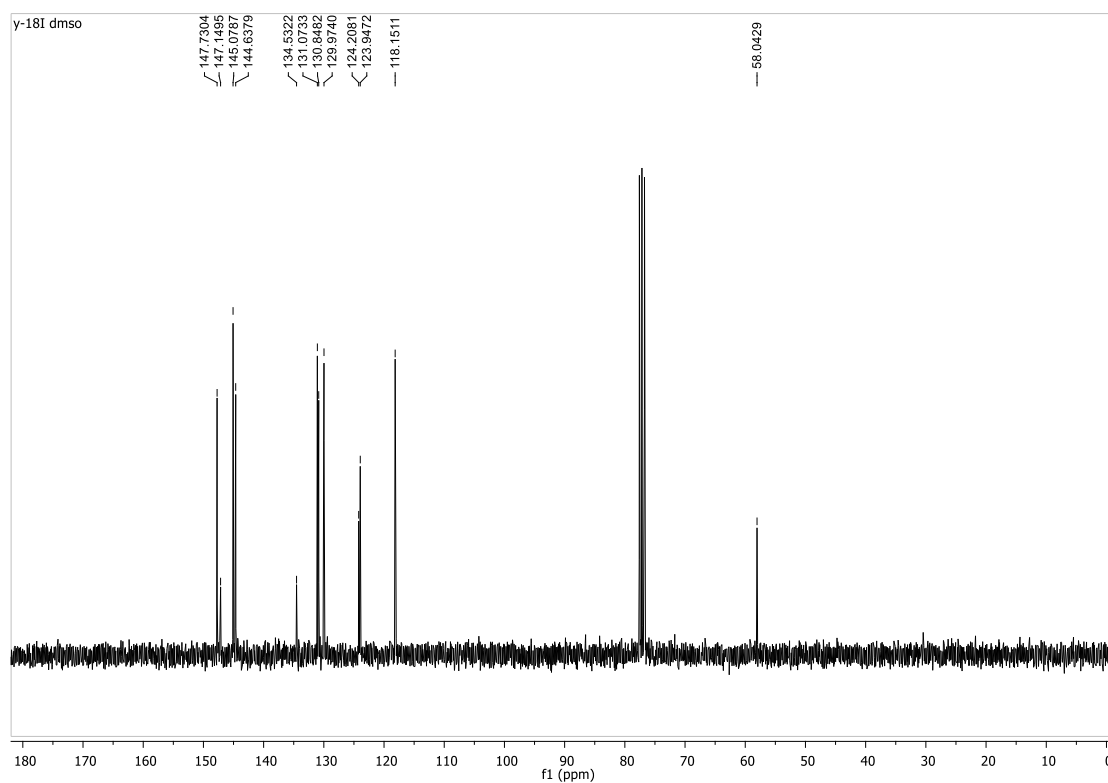
### 3-Iodo-1-(3-pyridyl)-1*H*-pyrrolo[2,3-*b*]pyridine (4h)



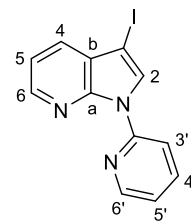
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



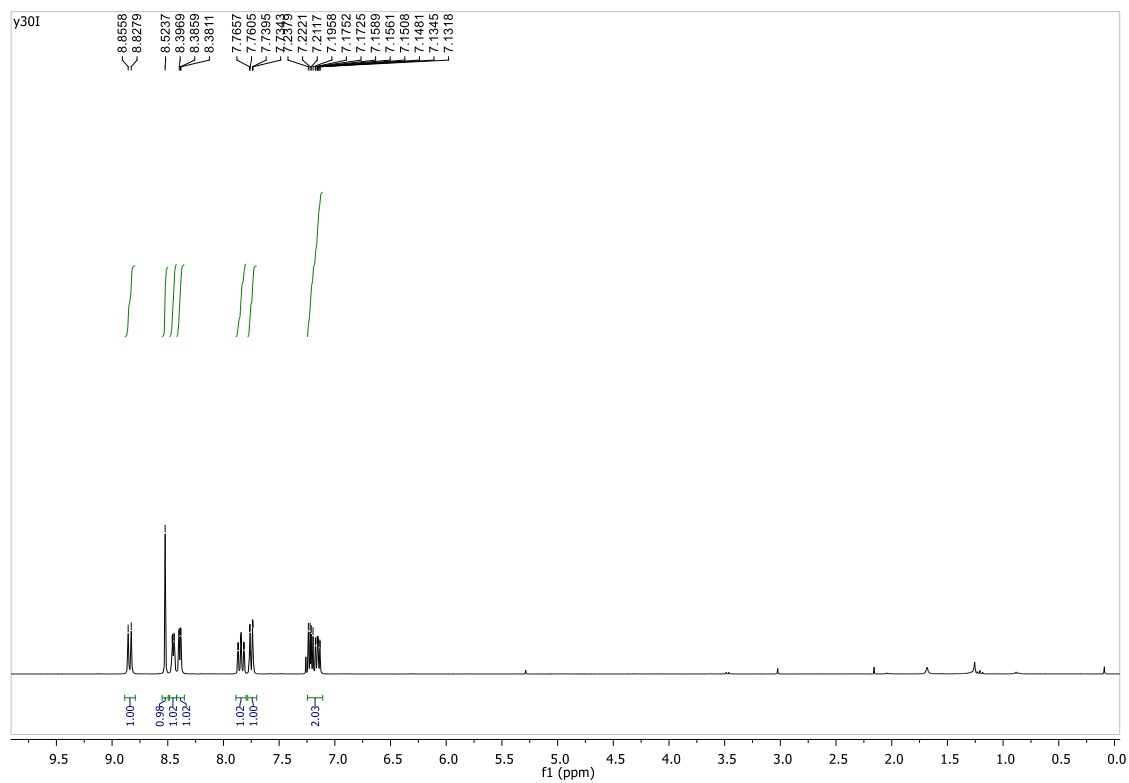
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



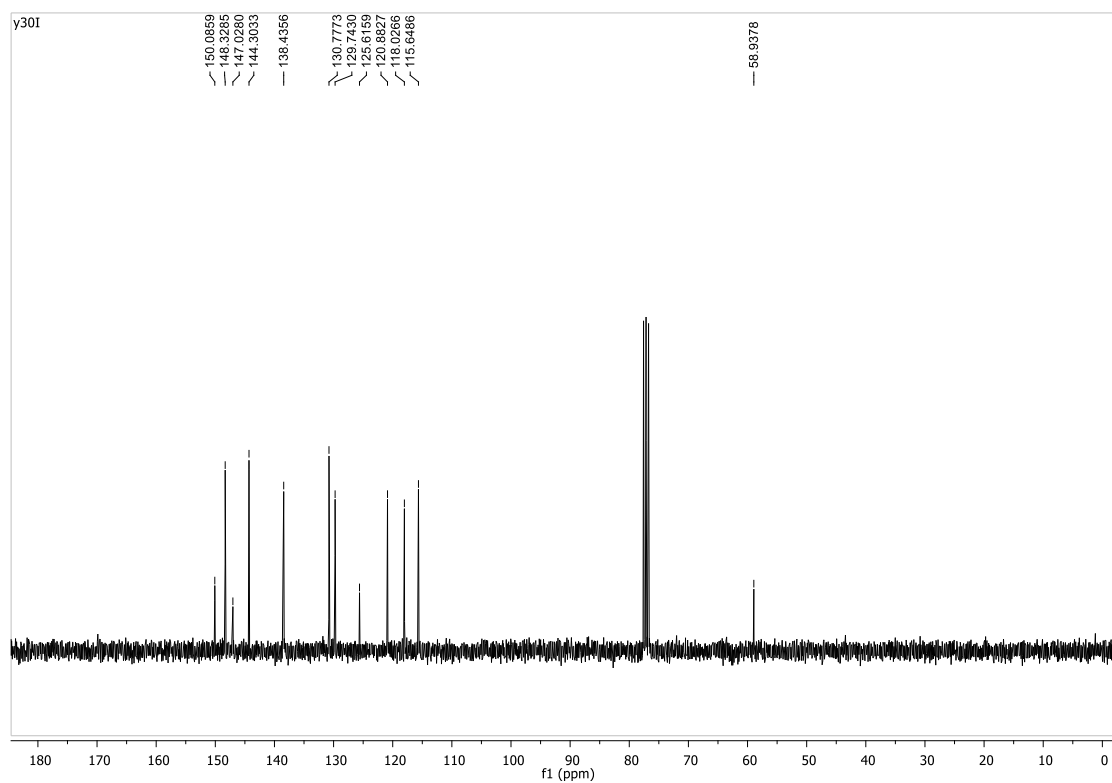
### 3-Iodo-1-(2-pyridyl)-1*H*-pyrrolo[2,3-*b*]pyridine (4i)



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )

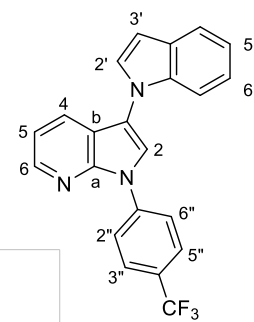
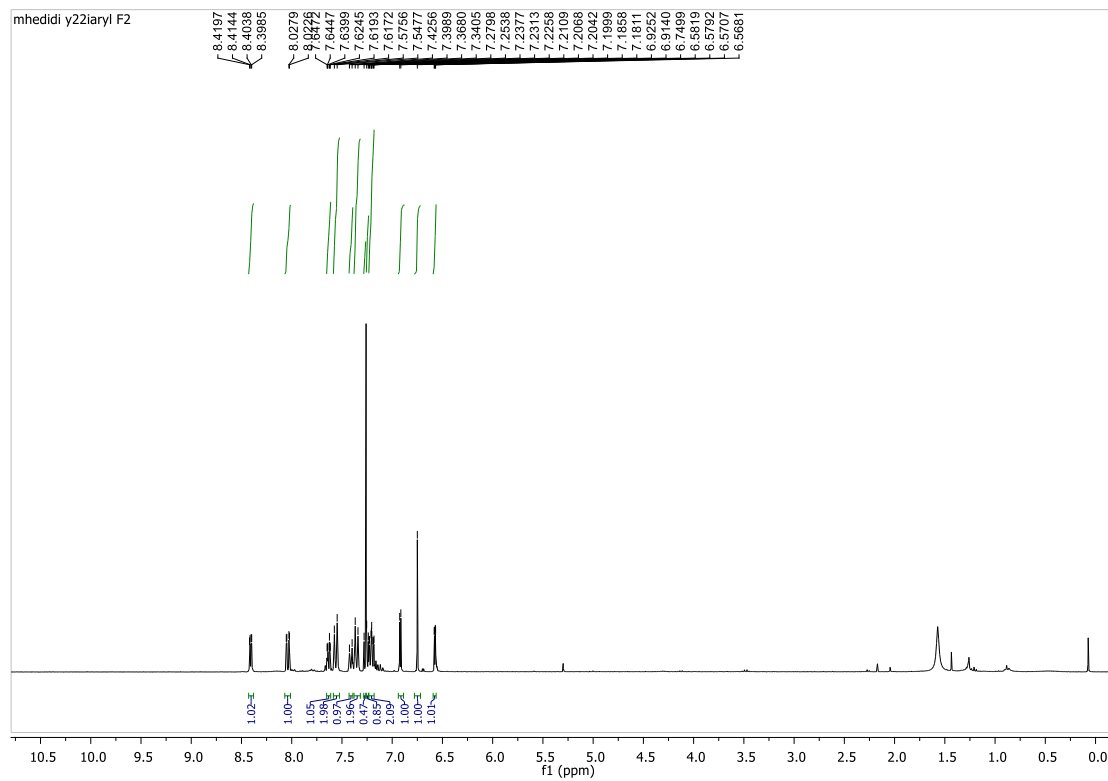


$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )

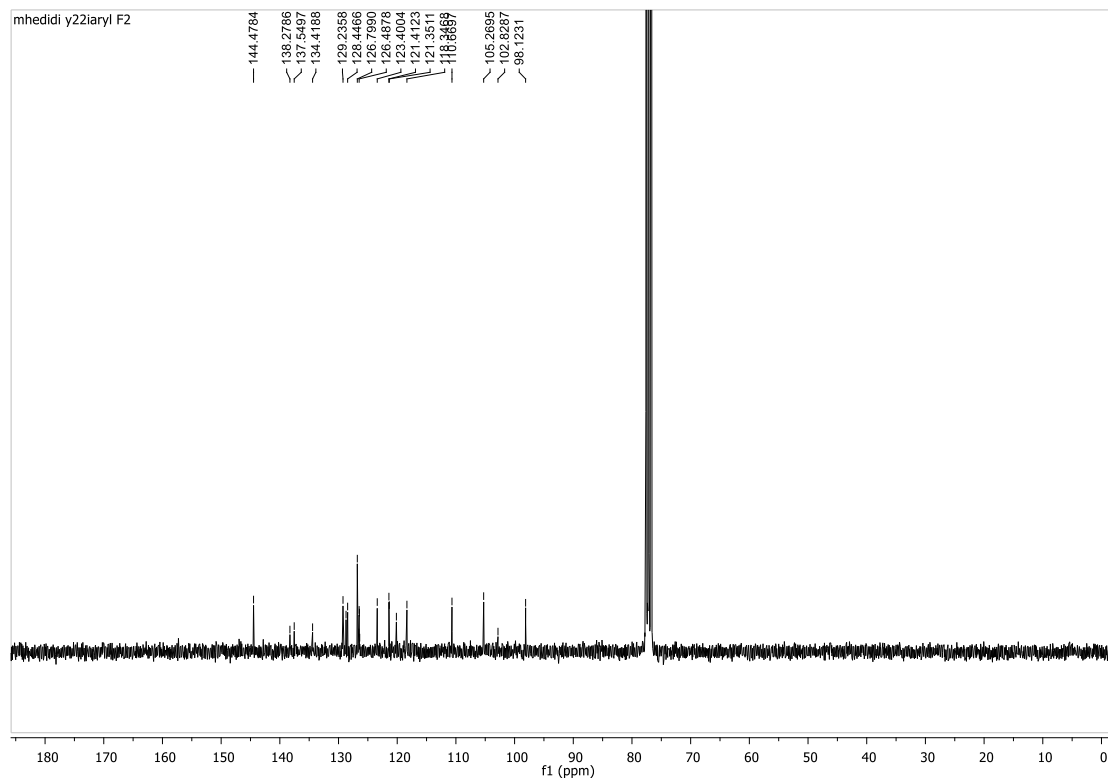


### 3-(1-Indolyl)-1-(4-(trifluoromethyl)phenyl)-1*H*-pyrrolo[2,3-*b*]pyridine (5e)

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)

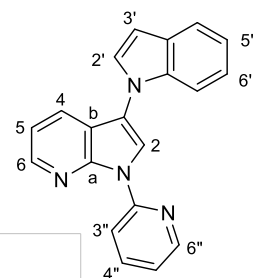
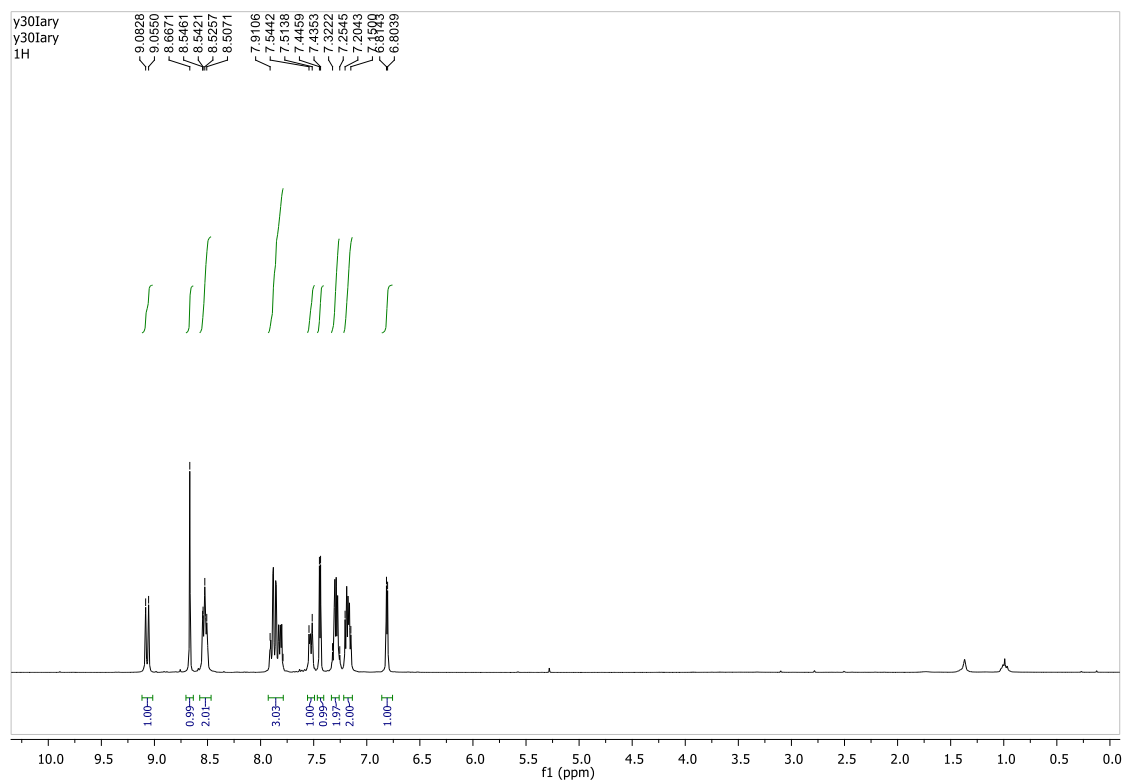


<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

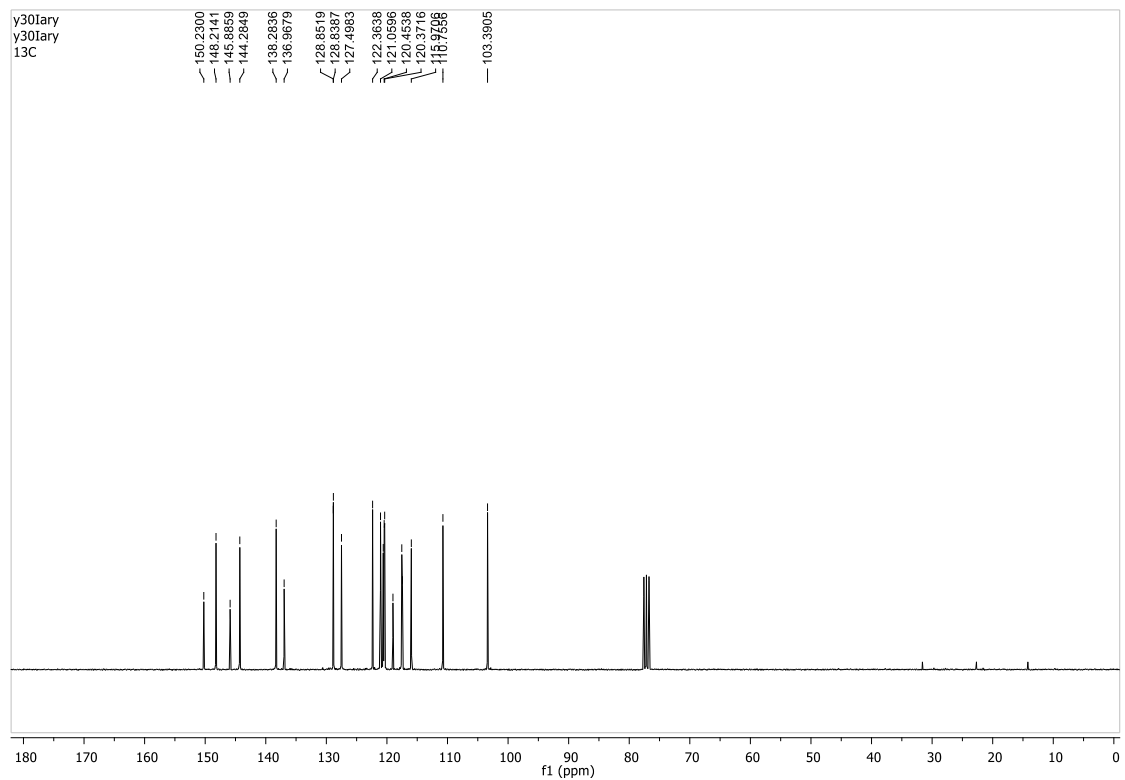


### 3-(1-Indolyl)-1-(2-pyridyl)-1*H*-pyrrolo[2,3-*b*]pyridine (5i)

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)

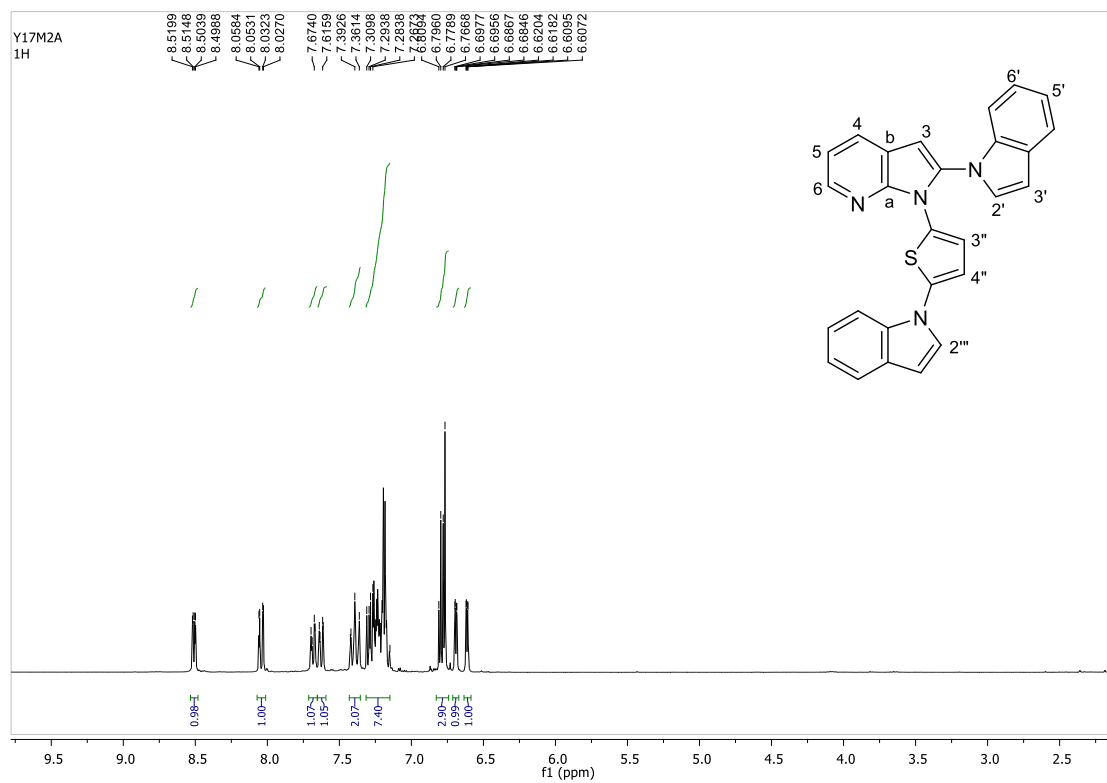


<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

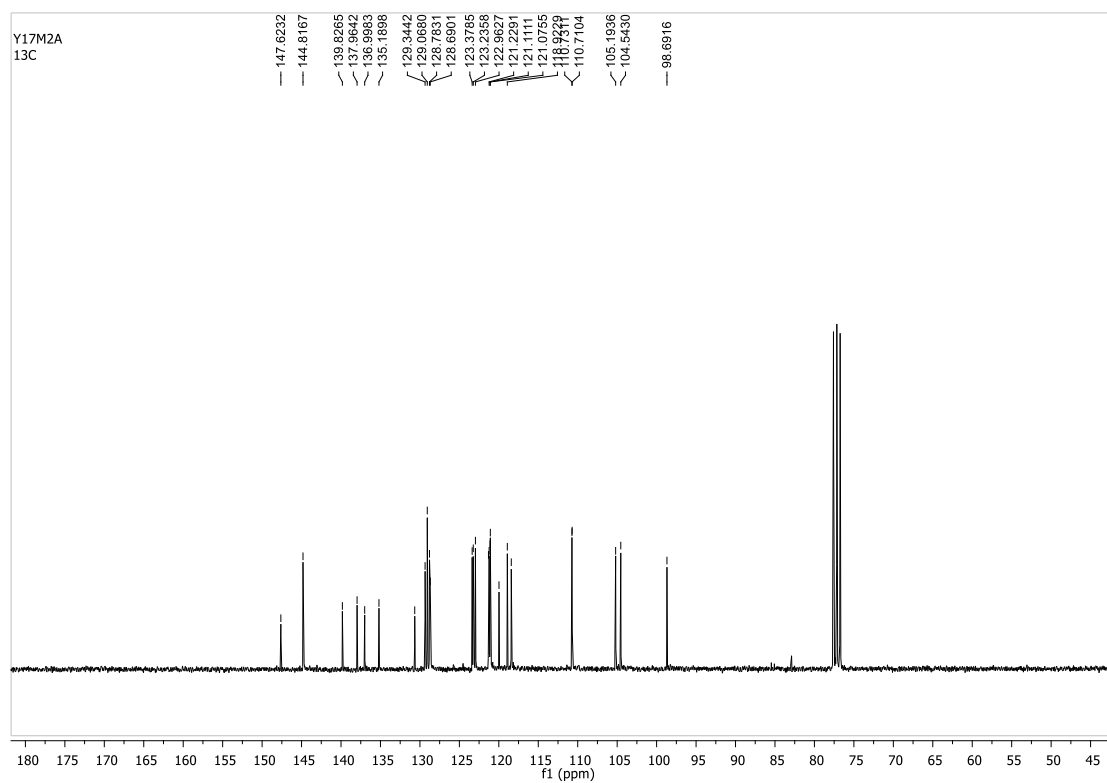


## 2-(1-Indolyl)-1-(5-(1-indolyl)-2-thienyl)-1*H*-pyrrolo[2,3-*b*]pyridine (6g')

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)



**Calculated values of the Gibbs energies  $\Delta G_{\text{acid}}$  [kJ·mol<sup>-1</sup>] for deprotonation**

