

Supporting Information

Exploration of Biaryl Carboxylic Acids as Proton Shuttles for the Selective Functionalization of Indole C–H Bonds

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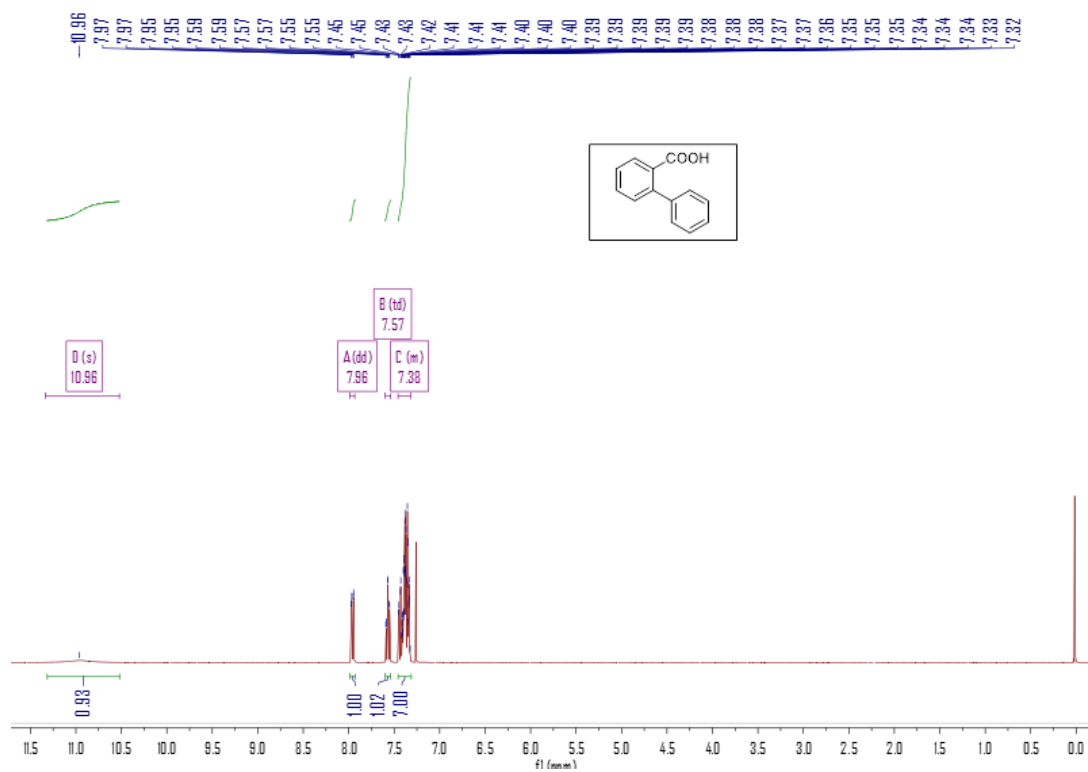
* E-Mail: fuyao@ustc.edu.cn

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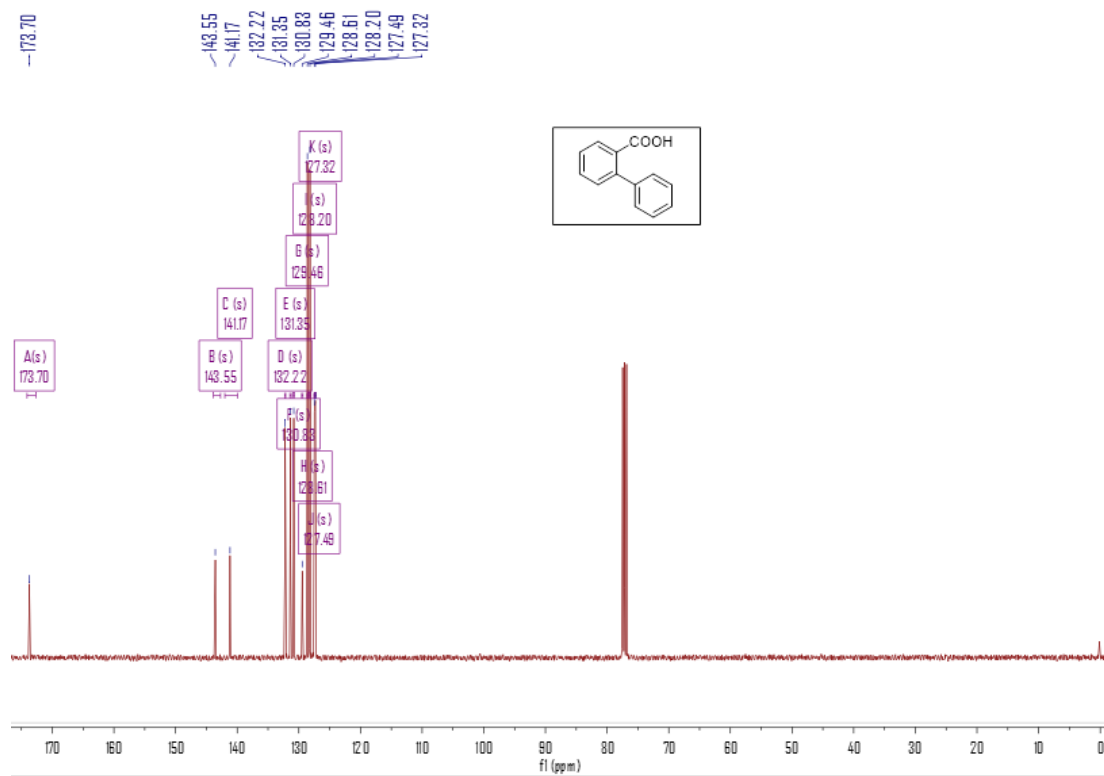
1. Spectral Data	S3
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1. Spectral Data

[1,1'-biphenyl]-2-carboxylic acid (**4b**)

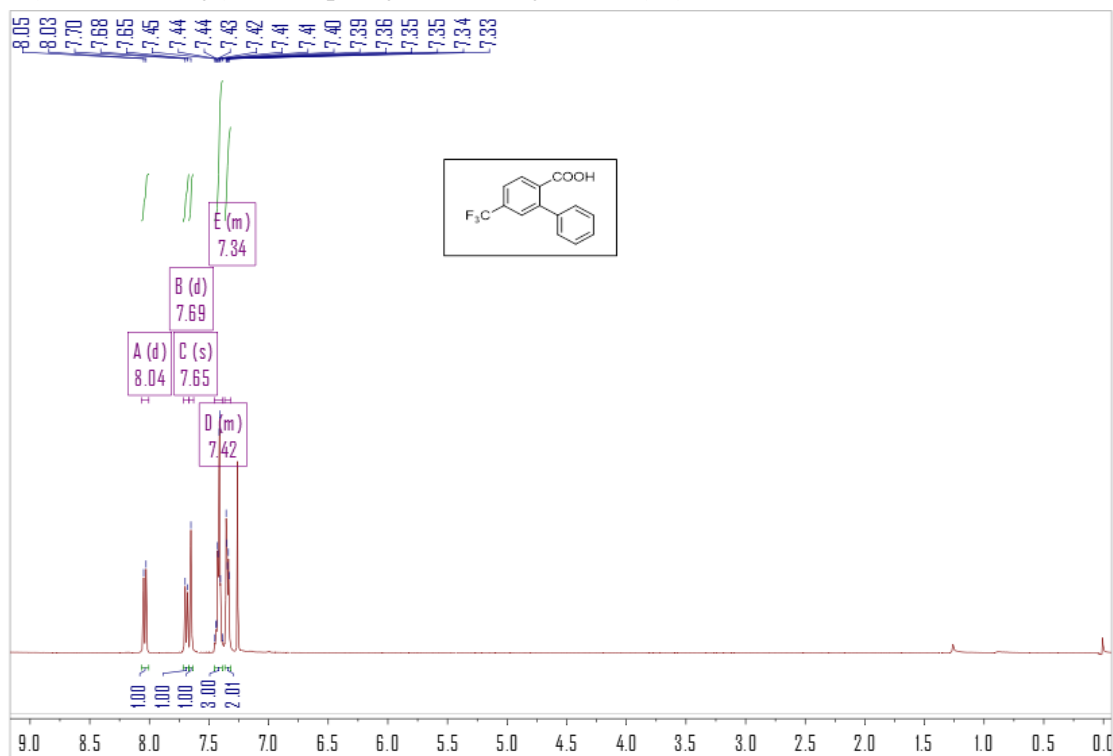


¹H NMR spectra for **4b**.

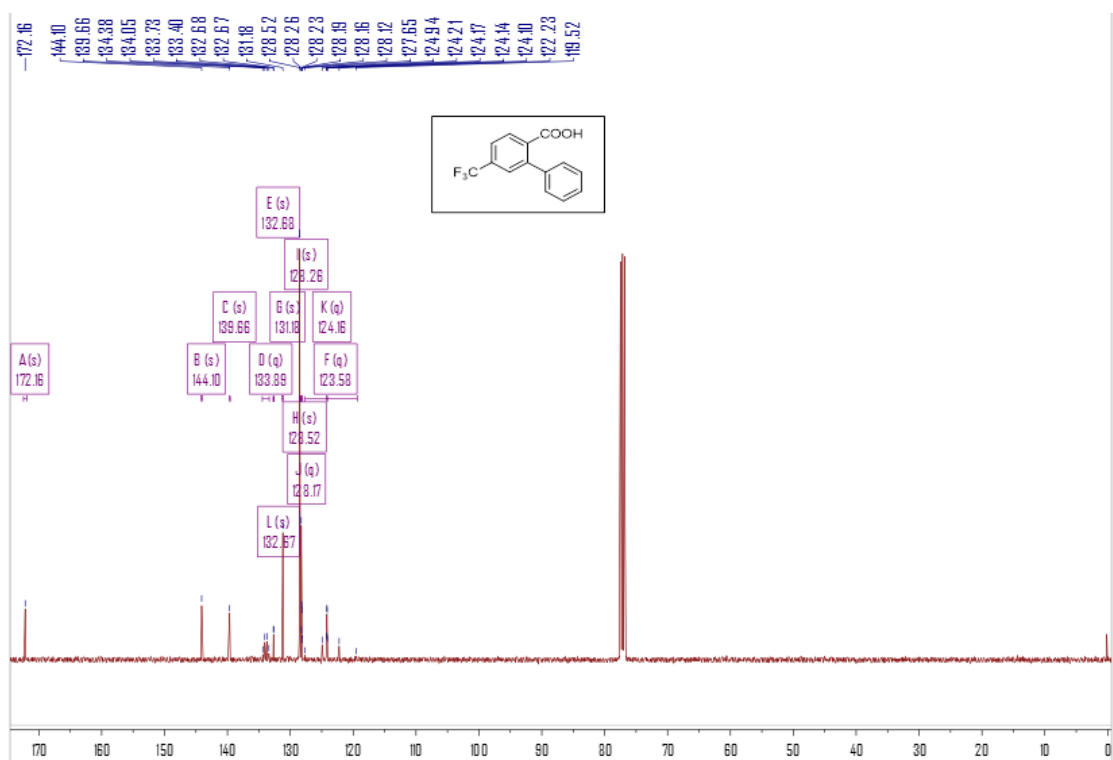


¹³C NMR spectra for **4b**.

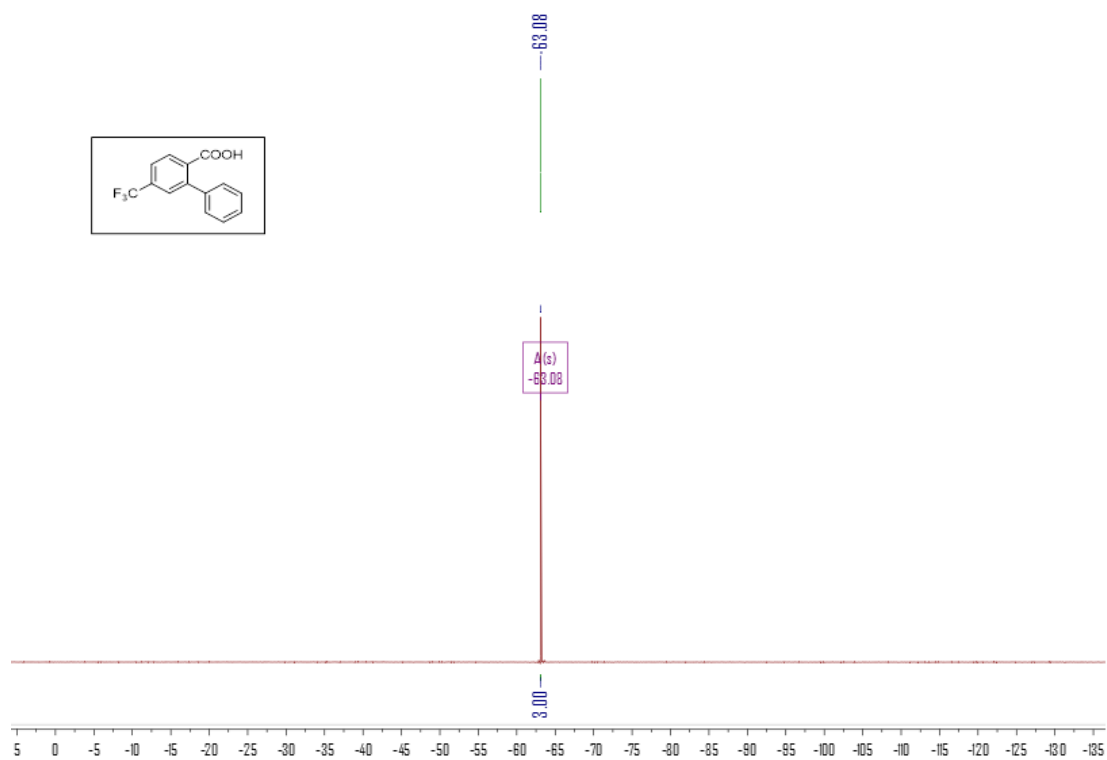
5-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid (4d)



¹H NMR spectra for **4d**.

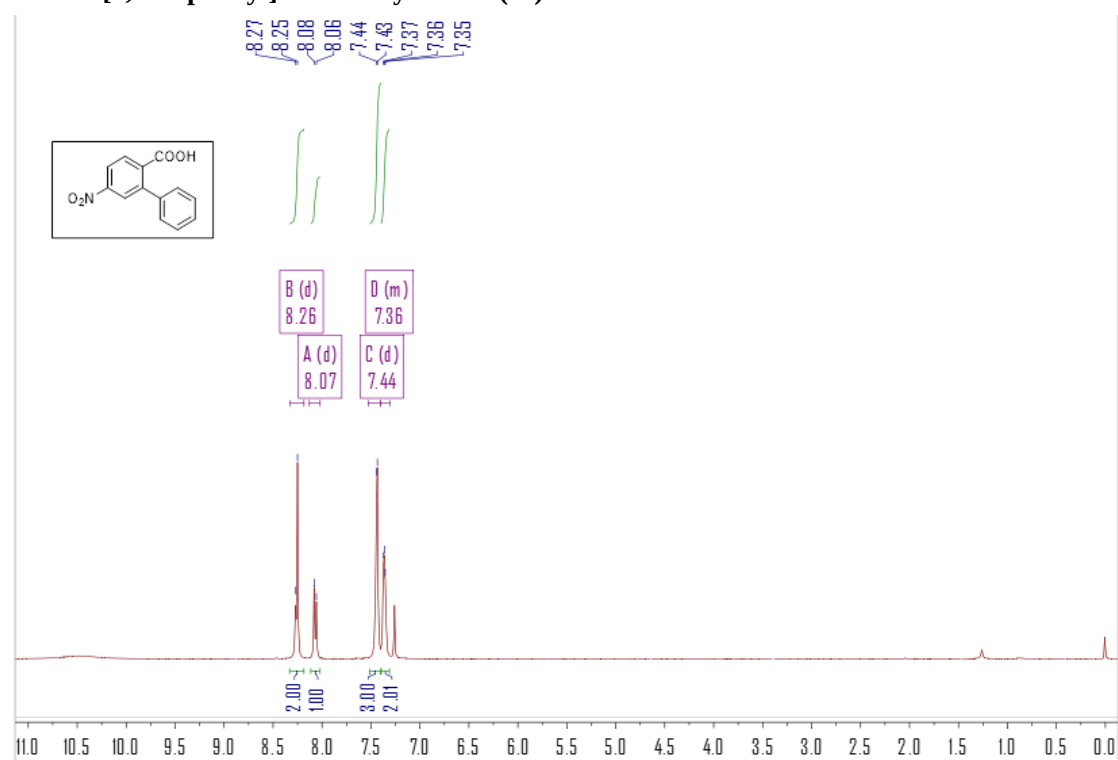


¹³C NMR spectra for **4d**.

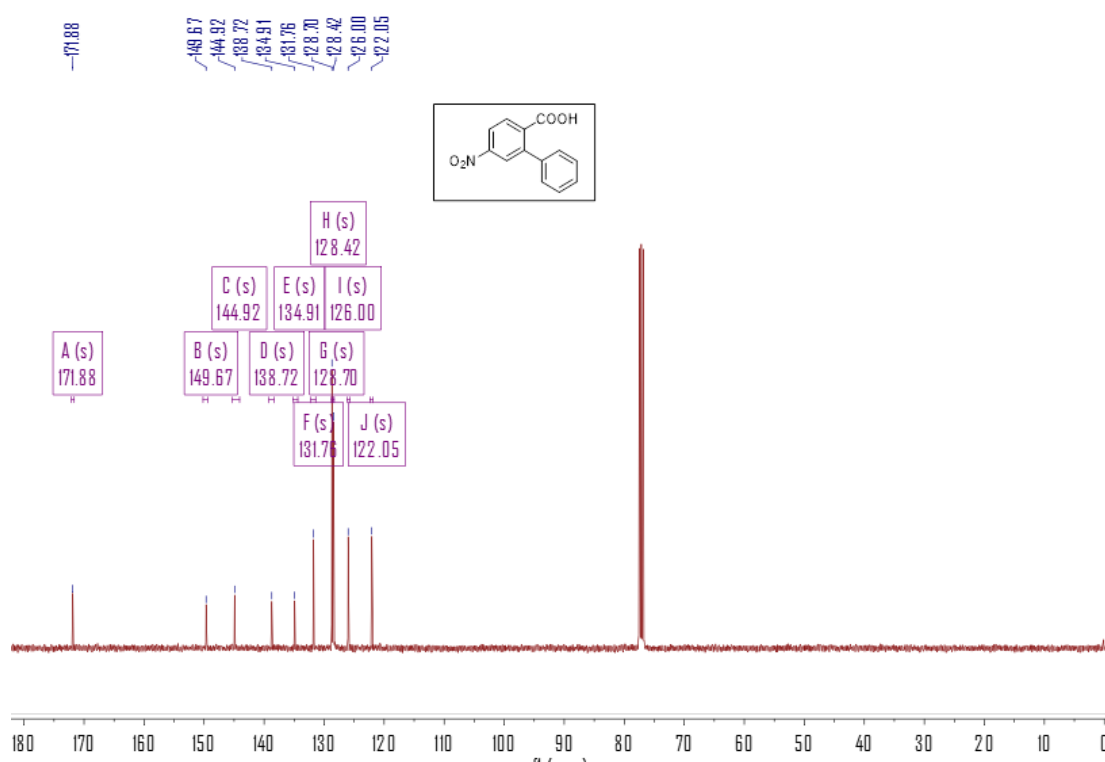


^{19}F NMR spectra for **4d**.

5-nitro-[1,1'-biphenyl]-2-carboxylic acid (4e**)**

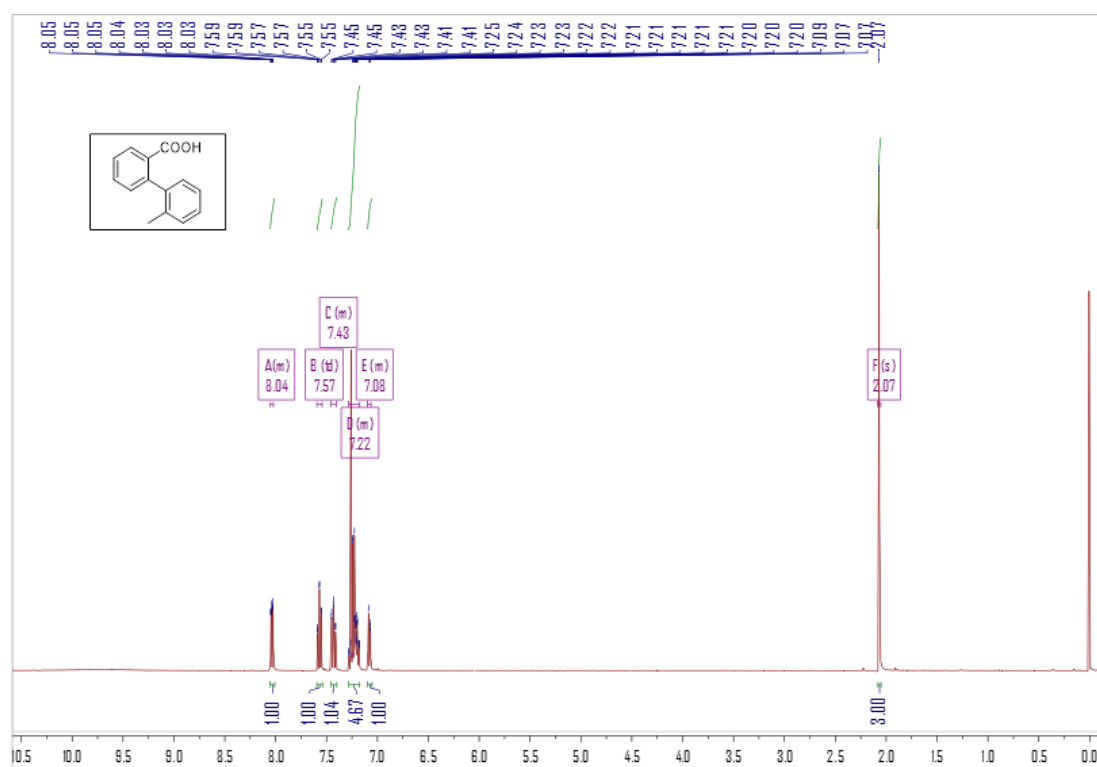


^1H NMR spectra for **4e**.

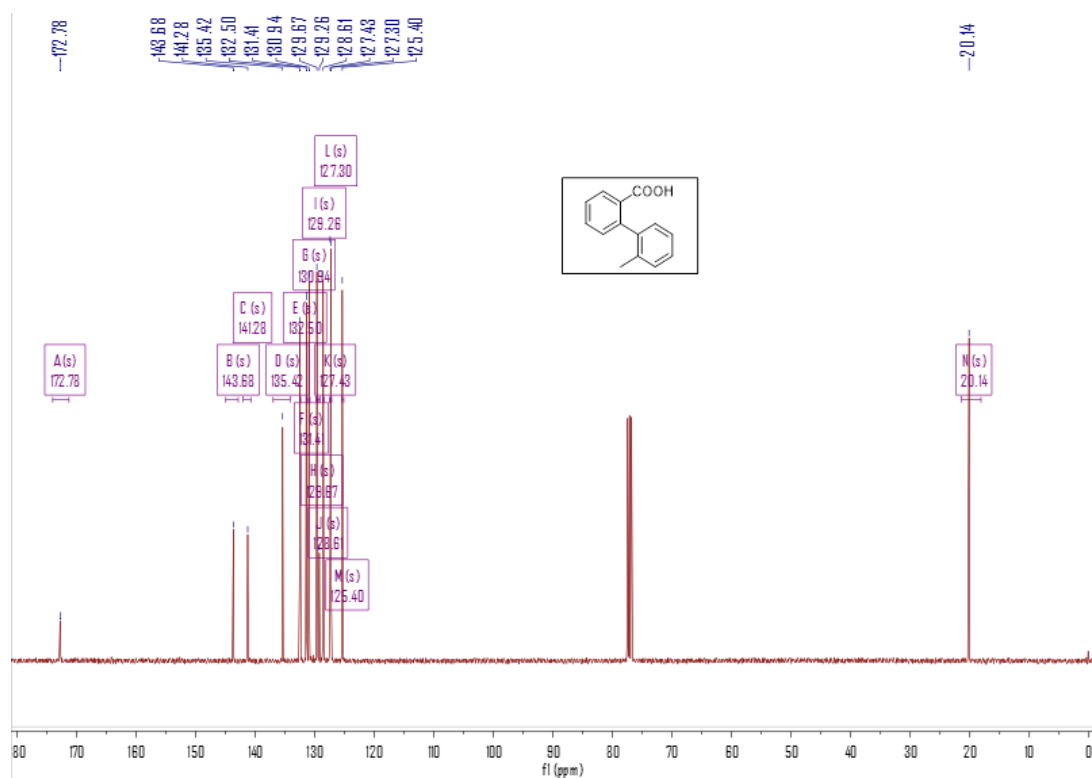


^{13}C NMR spectra for **4e**.

2'-methyl-[1,1'-biphenyl]-2-carboxylic acid (4f)

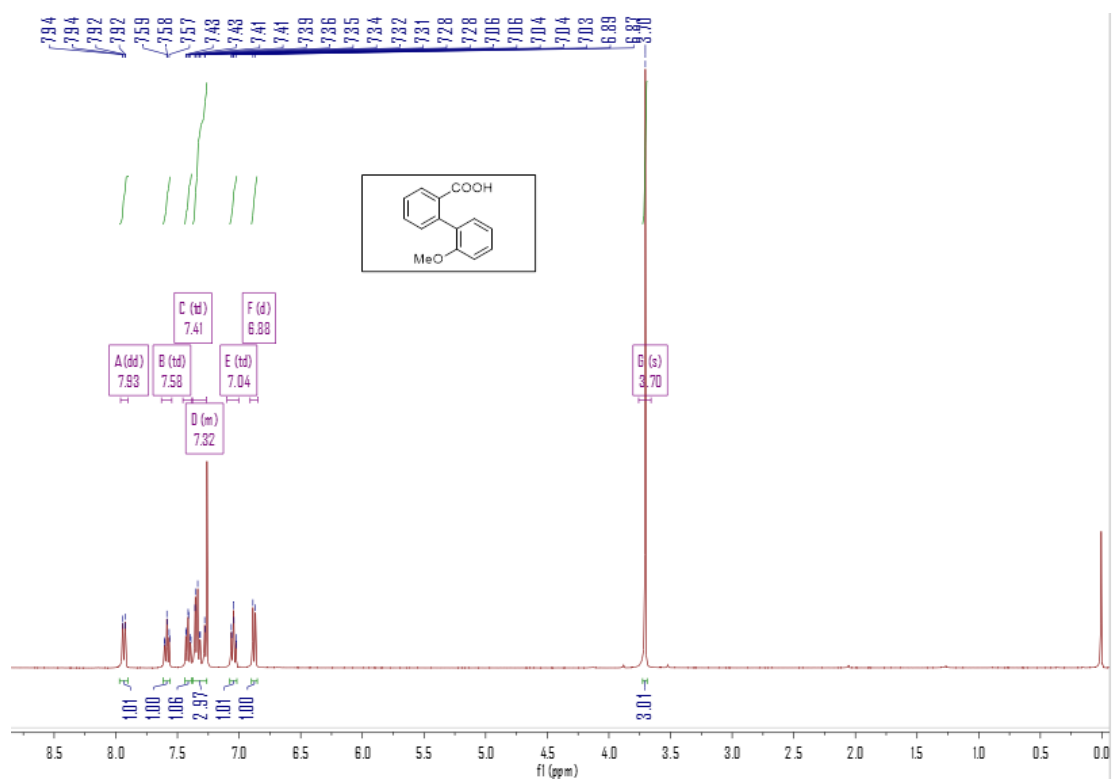


^1H NMR spectra for **4f**.

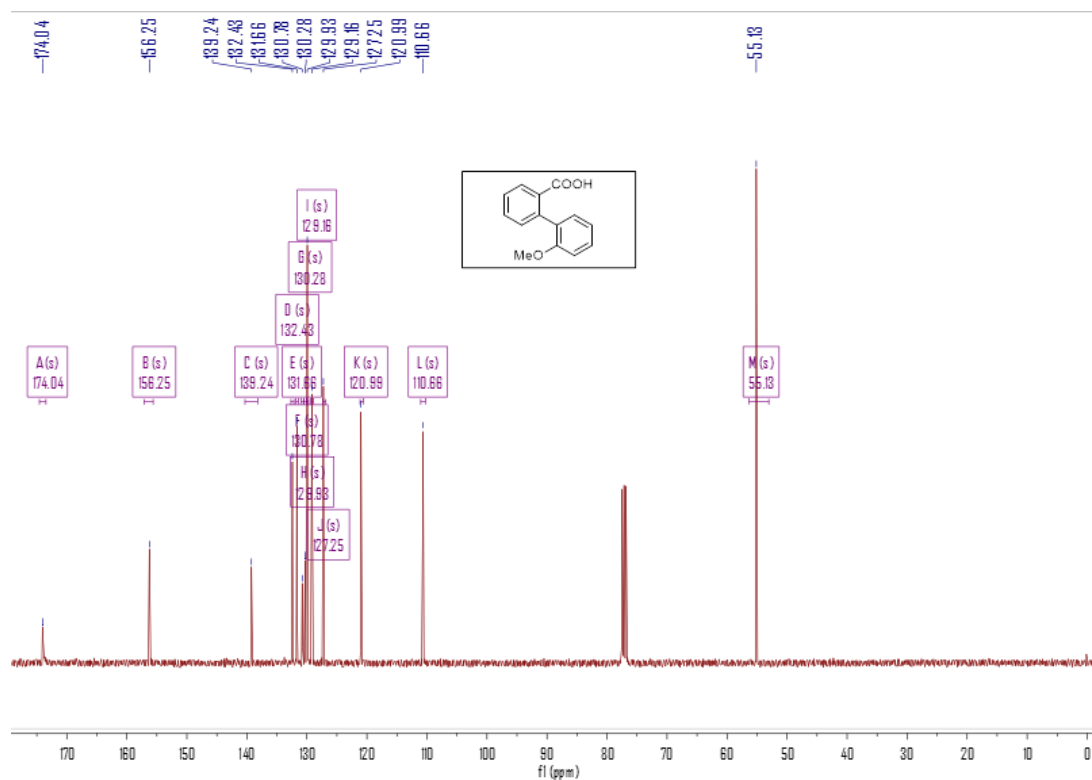


¹³C NMR spectra for **4f**.

2'-methoxy-[1,1'-biphenyl]-2-carboxylic acid (4g)

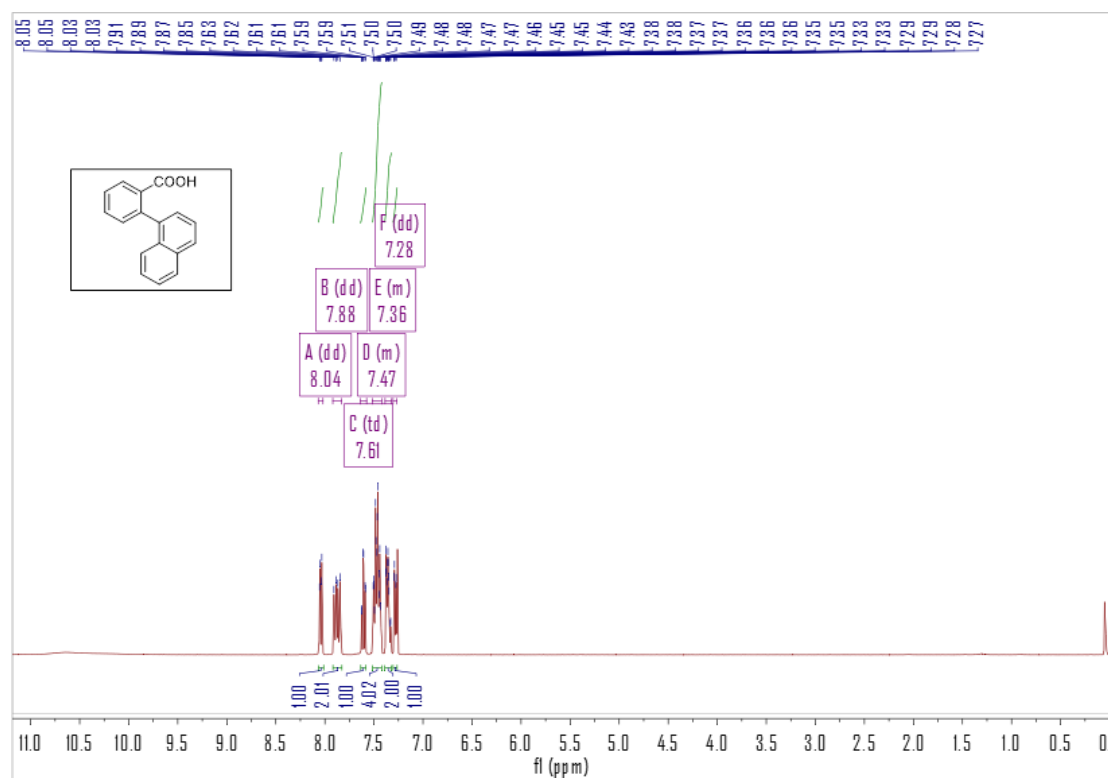


¹H NMR spectra for **4g**.

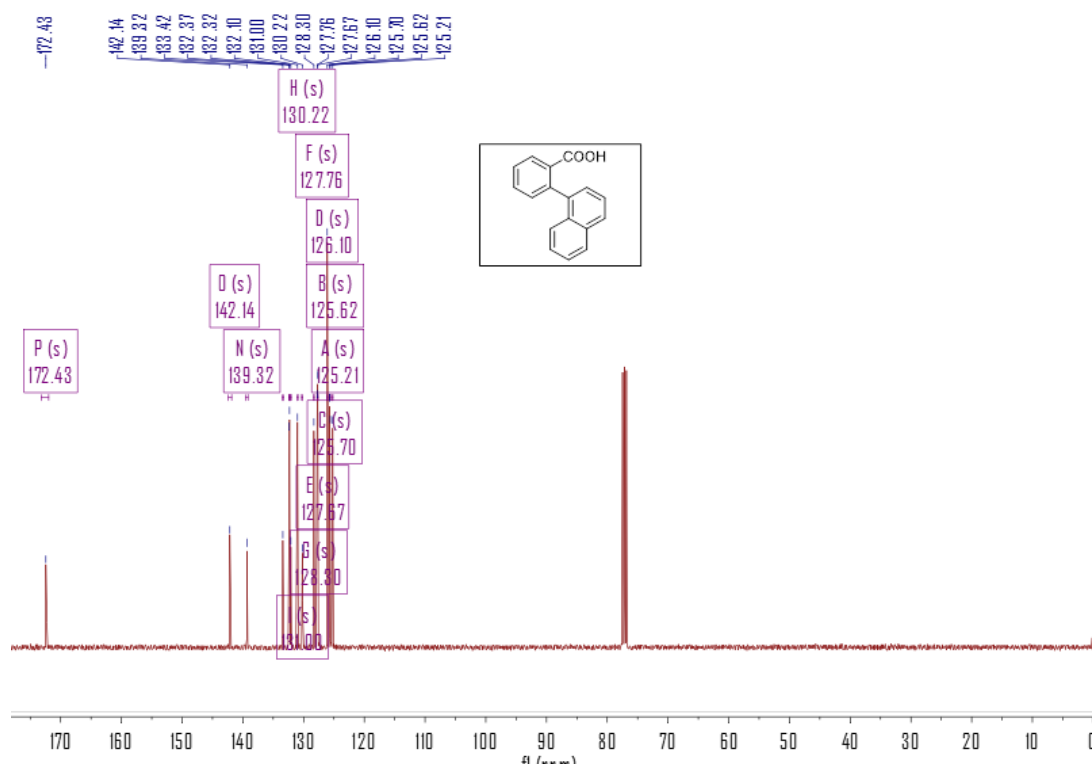


¹³C NMR spectra for **4g**.

2-(naphthalen-1-yl)benzoic acid (4h)

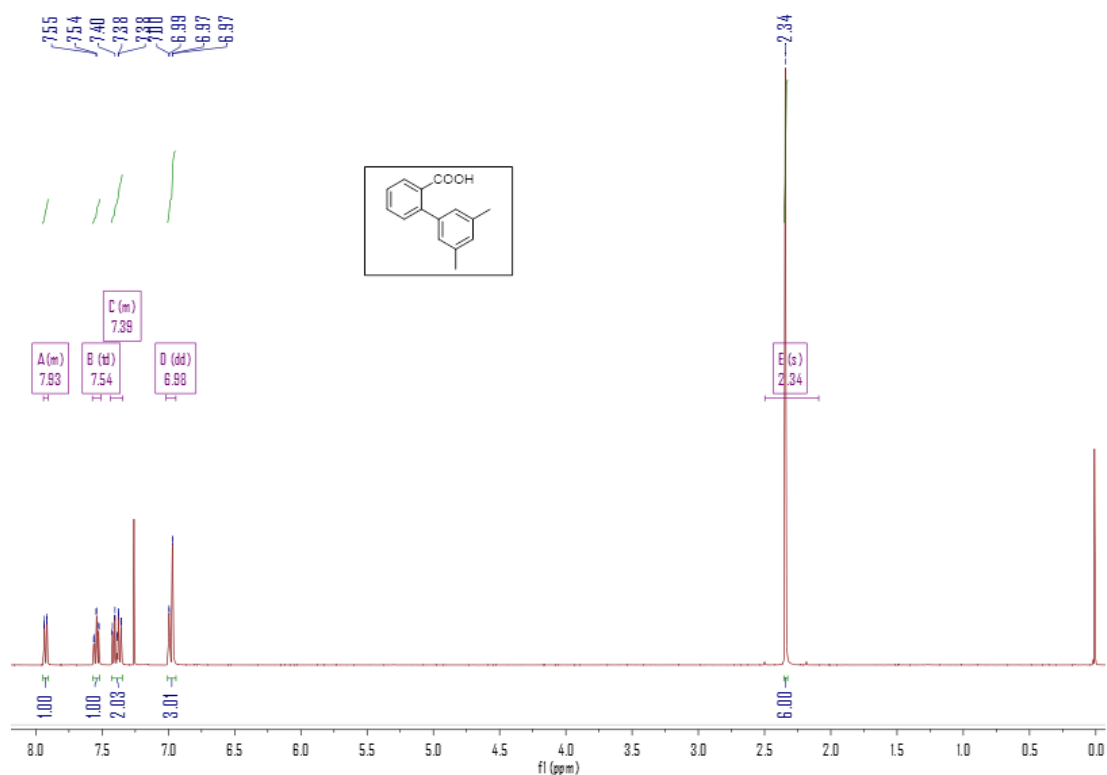


¹H NMR spectra for **4h**.

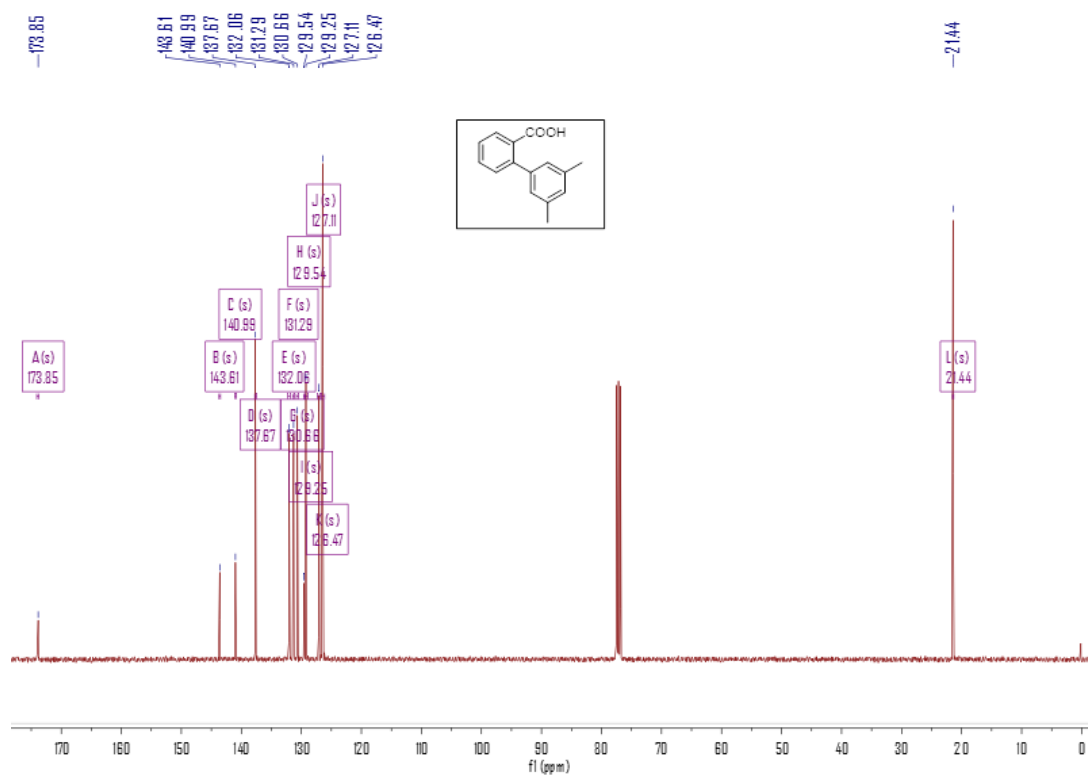


¹³C NMR spectra for **4h**.

3',5'-dimethyl-[1,1'-biphenyl]-2-carboxylic acid (4i)

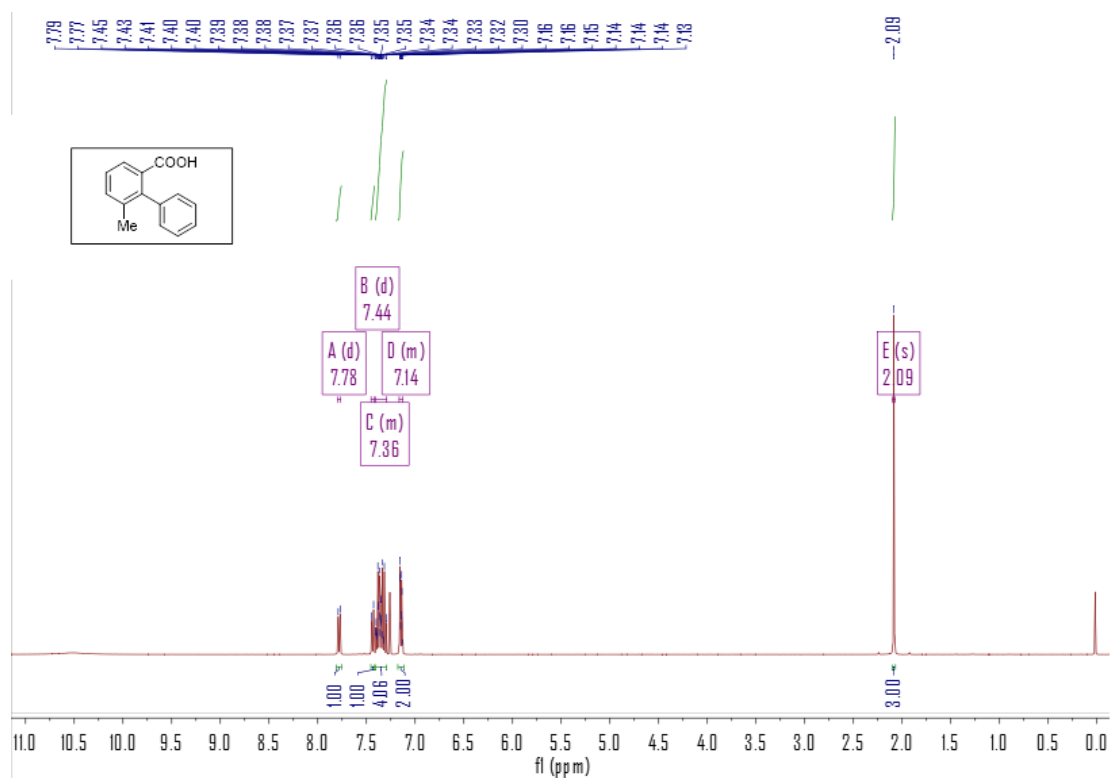


¹H NMR spectra for **4i**.

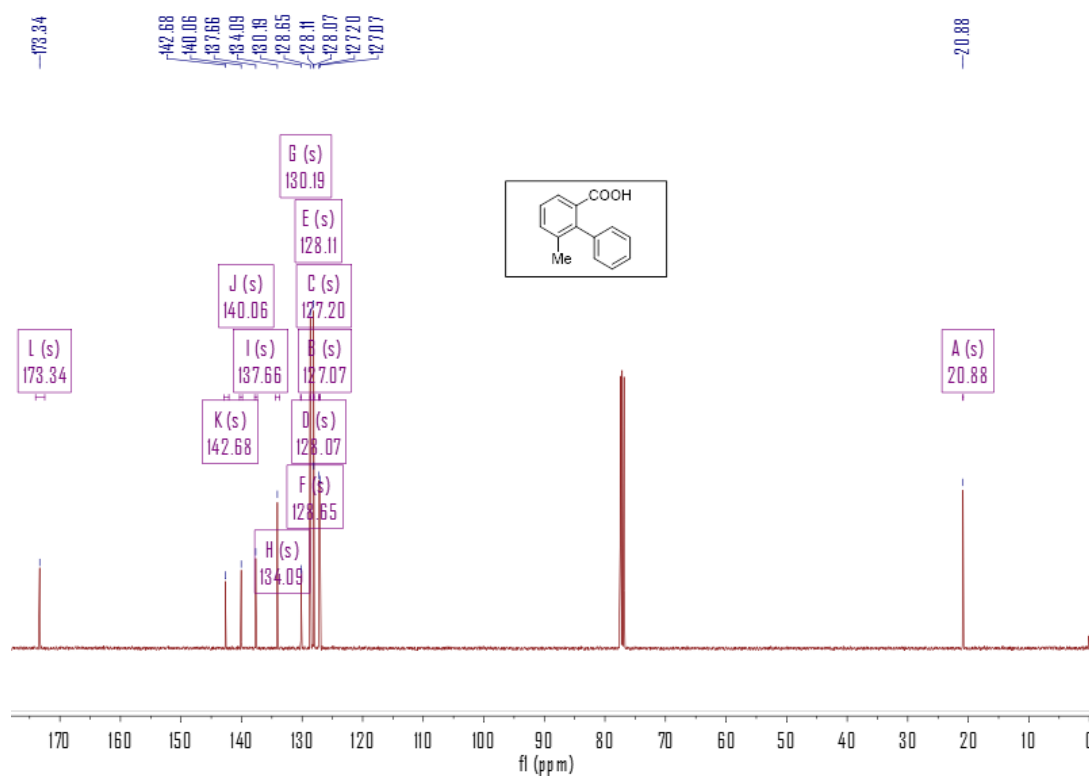


¹³C NMR spectra for **4i**.

6-methyl-[1,1'-biphenyl]-2-carboxylic acid (4k)

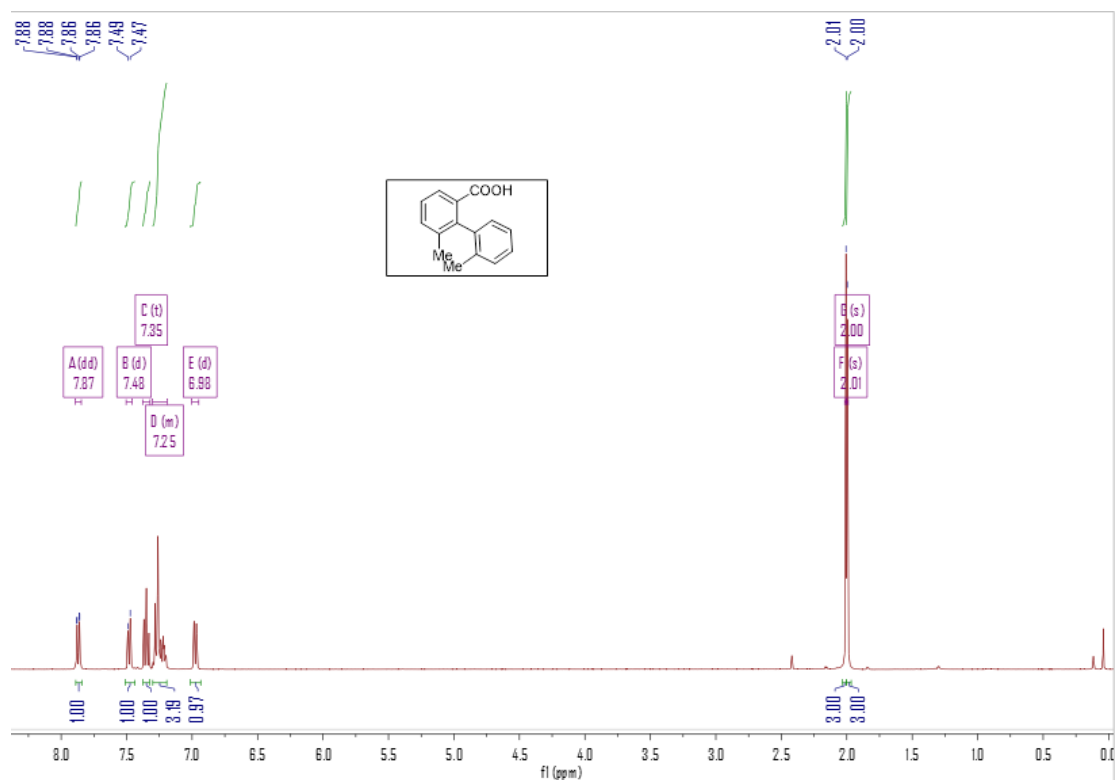


¹H NMR spectra for **4k**.

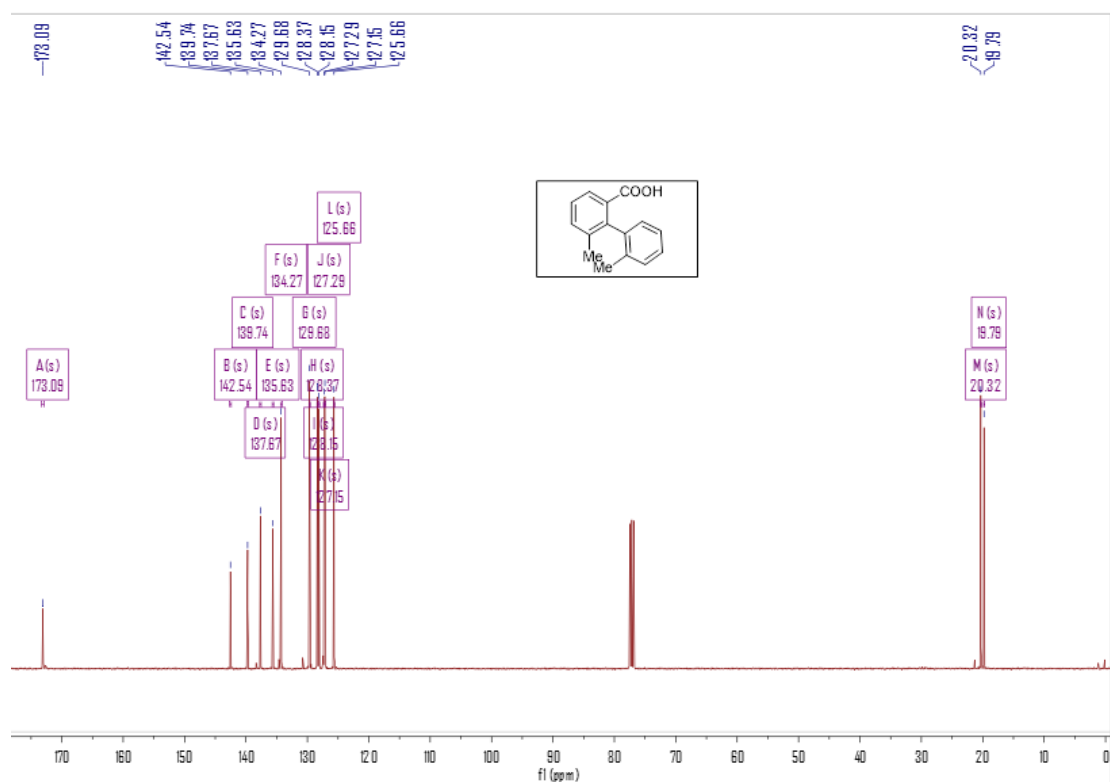


¹³C NMR spectra for **4k**.

2',6-dimethyl-1,1'-biphenyl-2-carboxylic acid (4l)

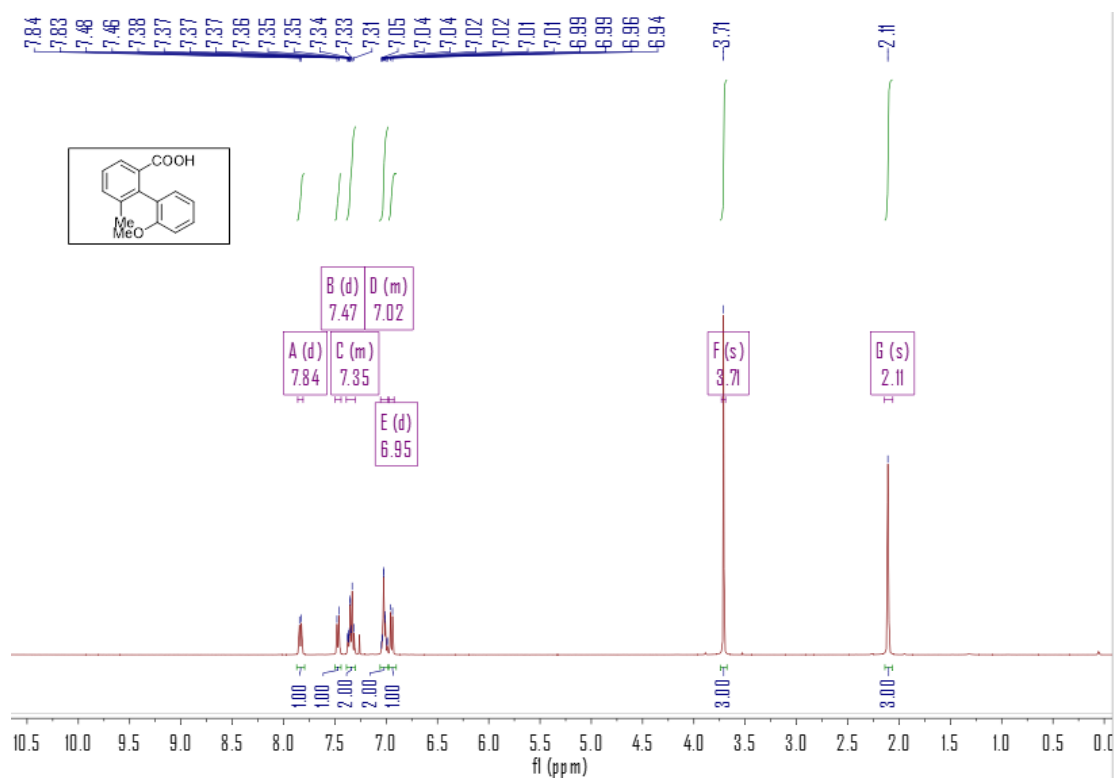


¹H NMR spectra for **4l**.

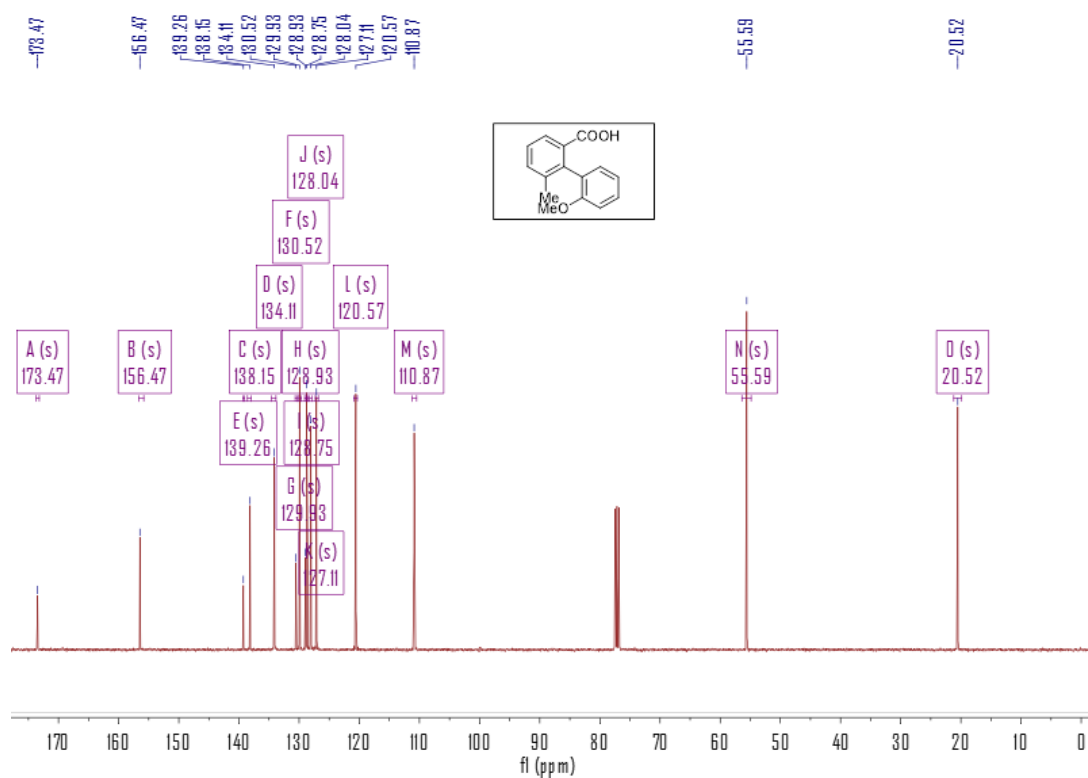


¹³C NMR spectra for **4l**.

2'-methoxy-6-methyl-[1,1'-biphenyl]-2-carboxylic acid (4m)

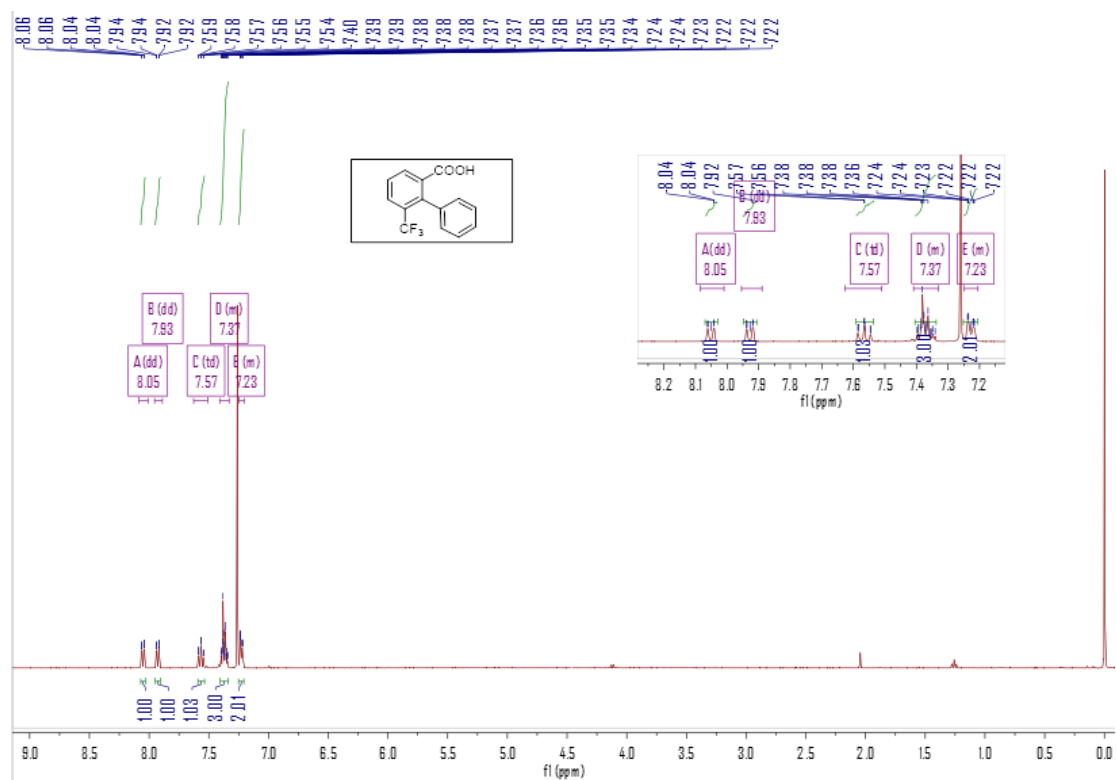


¹H NMR spectra for **4m**.

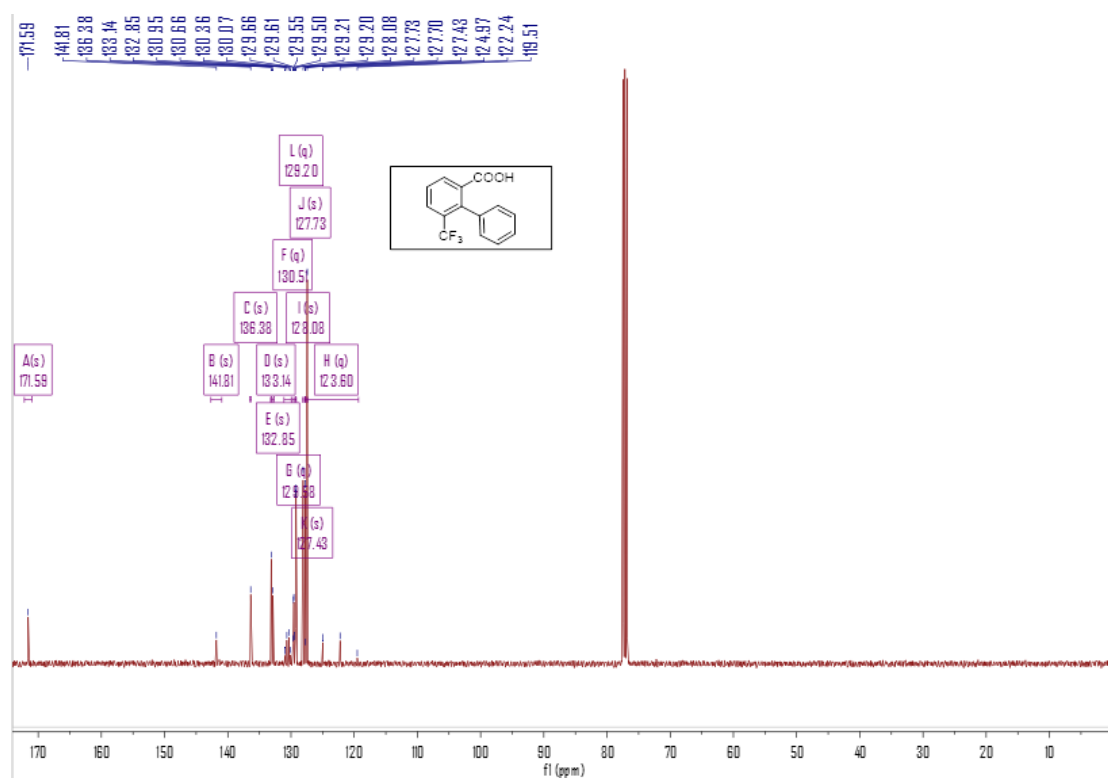


¹³C NMR spectra for **4m**.

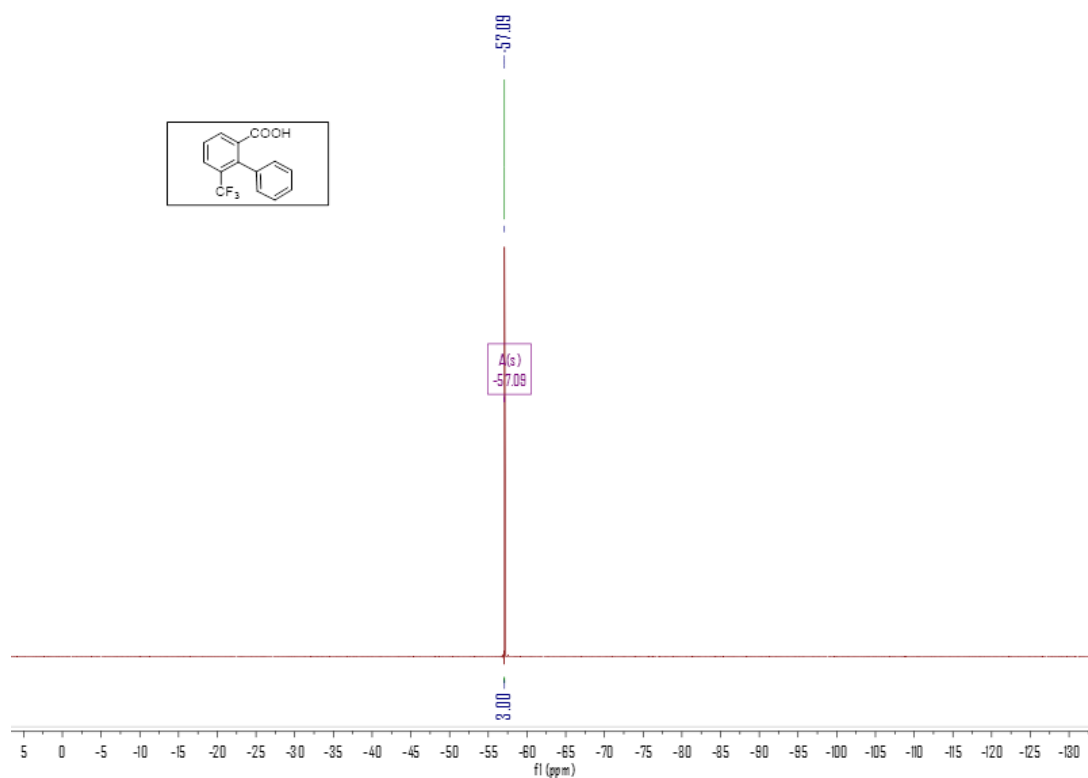
6-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid (4n)



¹H NMR spectra for **4n**.

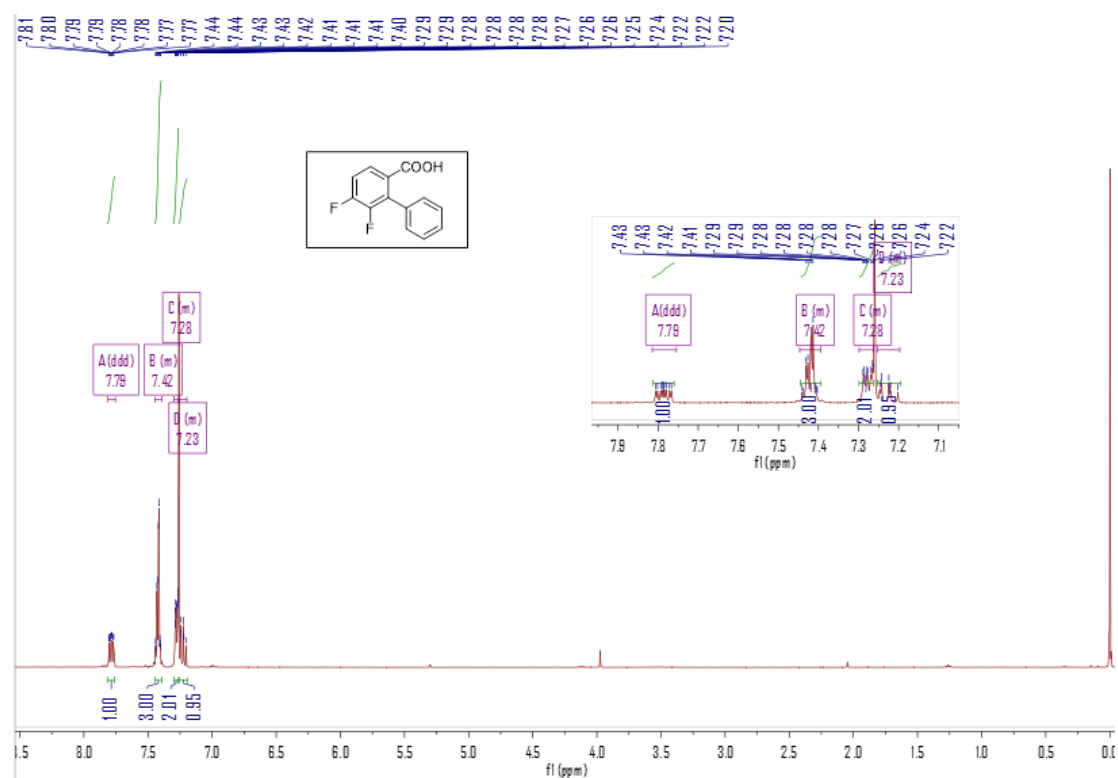


¹³C NMR spectra for 4n.

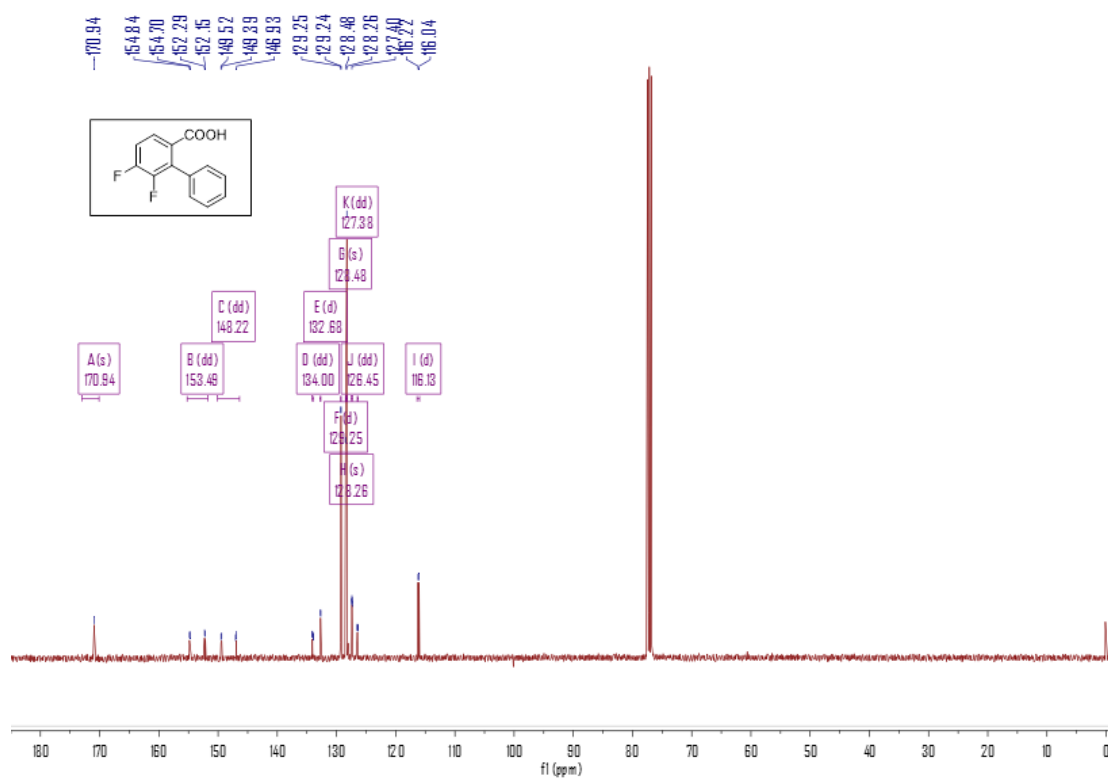


¹⁹F NMR spectra for 4n.

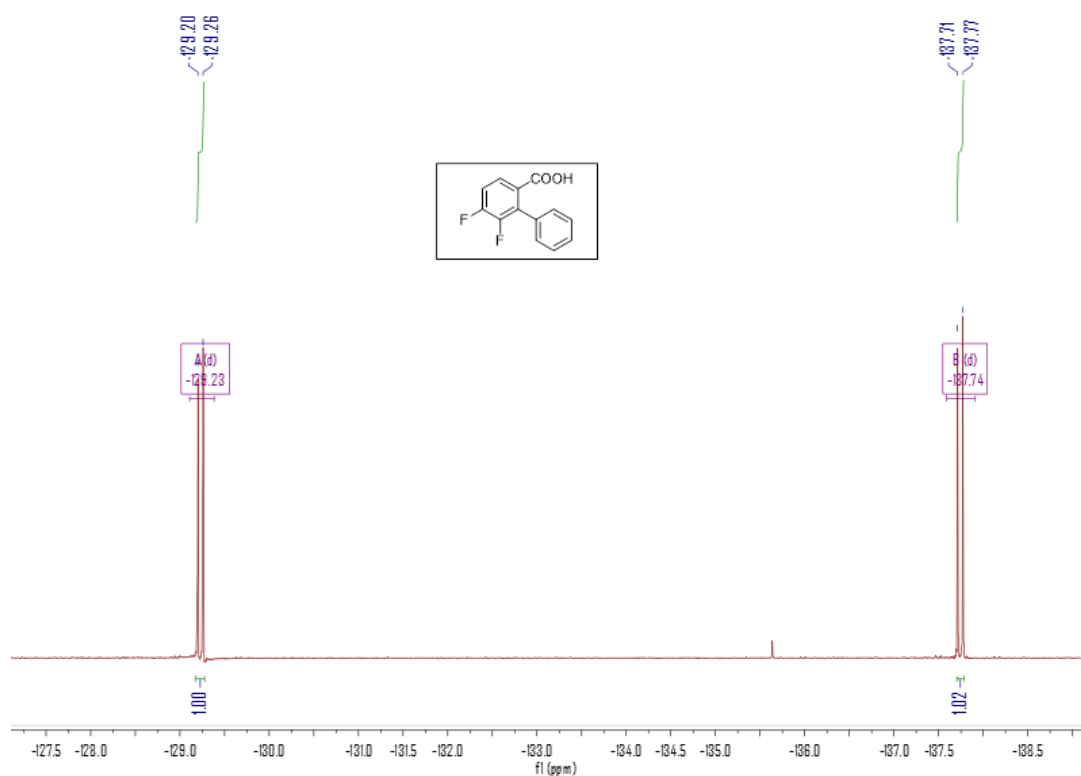
5,6-difluoro-[1,1'-biphenyl]-2-carboxylic acid (4o)



¹H NMR spectra for **4o**.

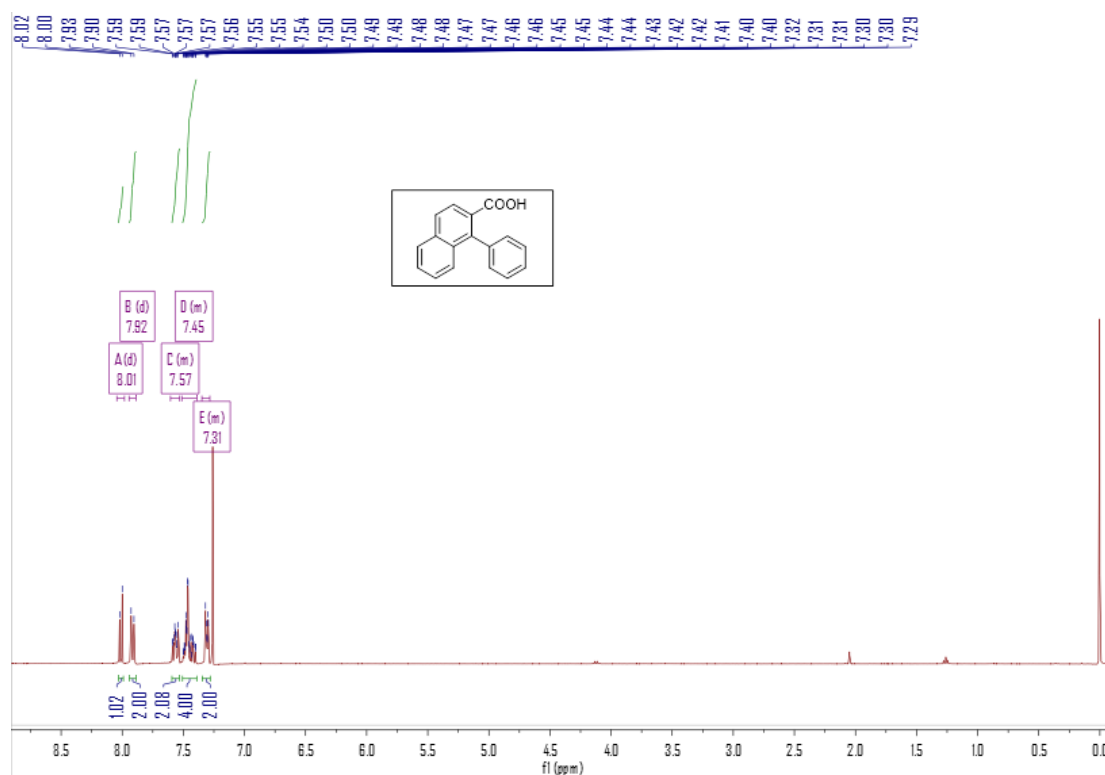


¹³C NMR spectra for **4o**.

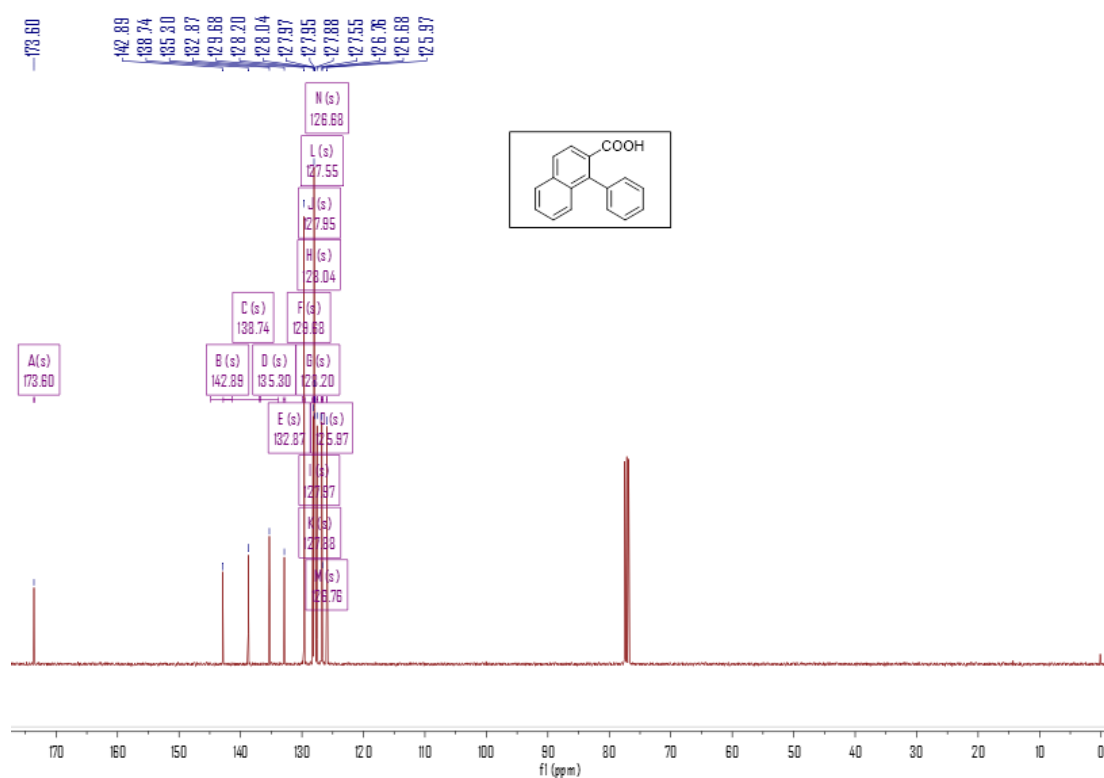


^{19}F NMR spectra for 4o.

1-phenyl-2-naphthoic acid (4p)

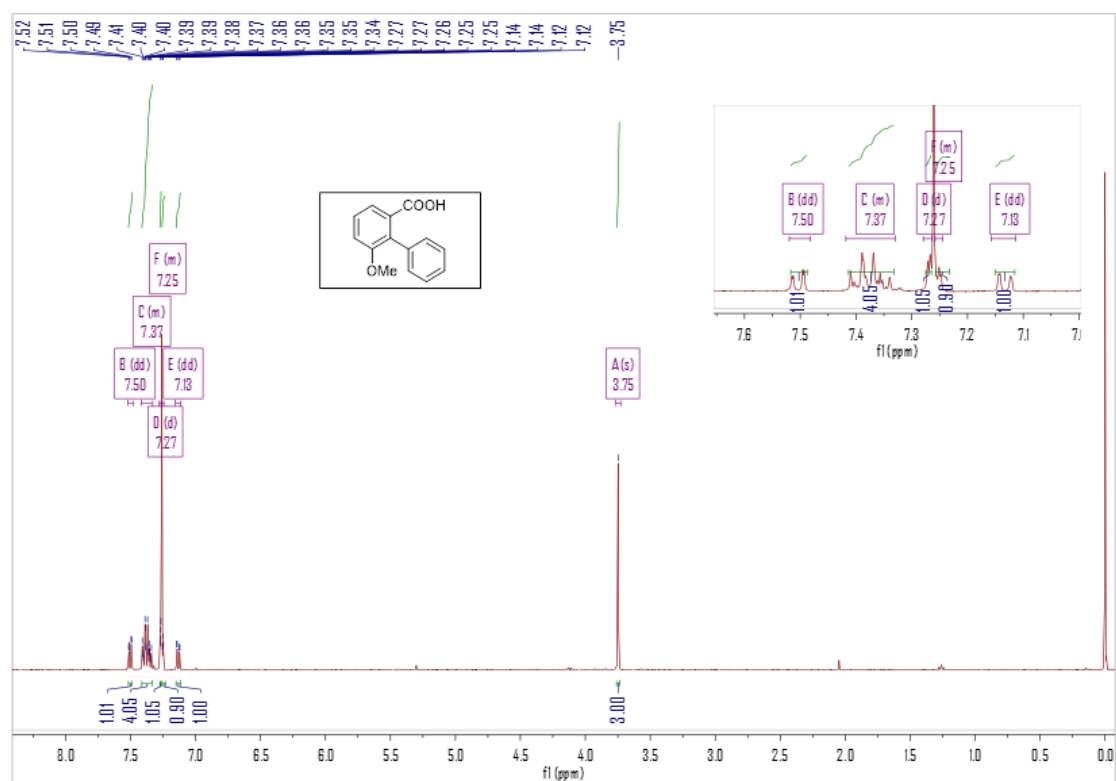


^1H NMR spectra for 4p.

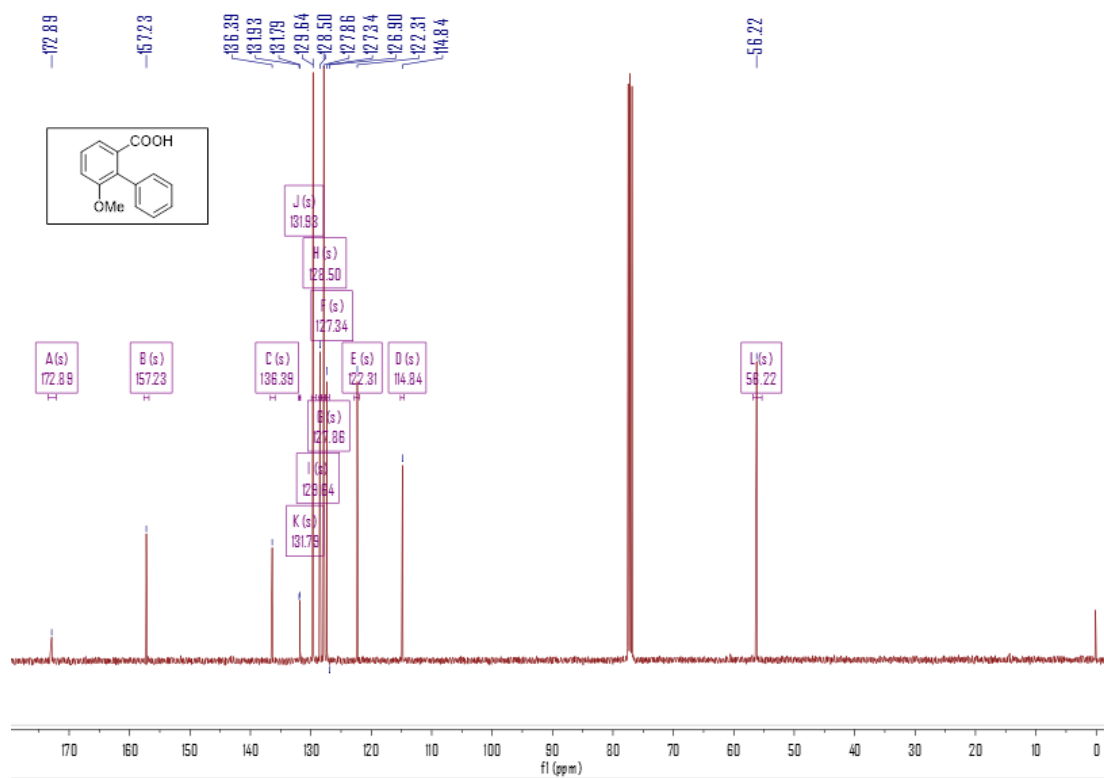


¹³C NMR spectra for **4p**.

6-methoxy-[1,1'-biphenyl]-2-carboxylic acid (4q)

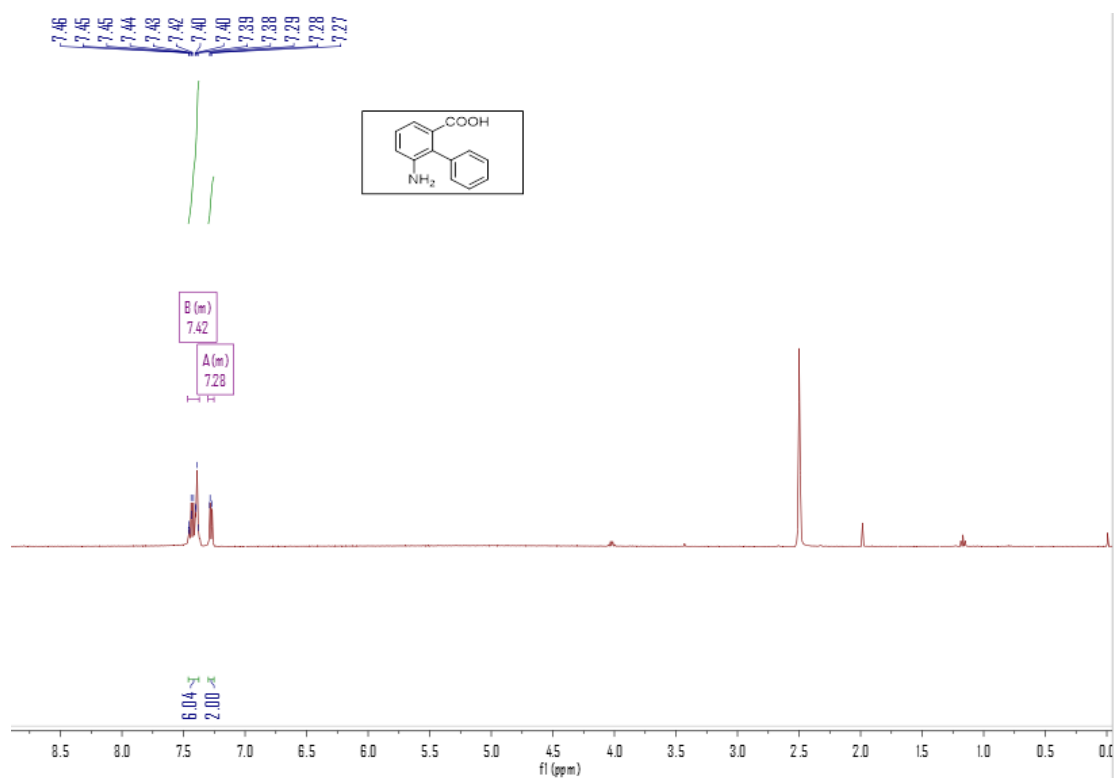


¹H NMR spectra for **4q**.

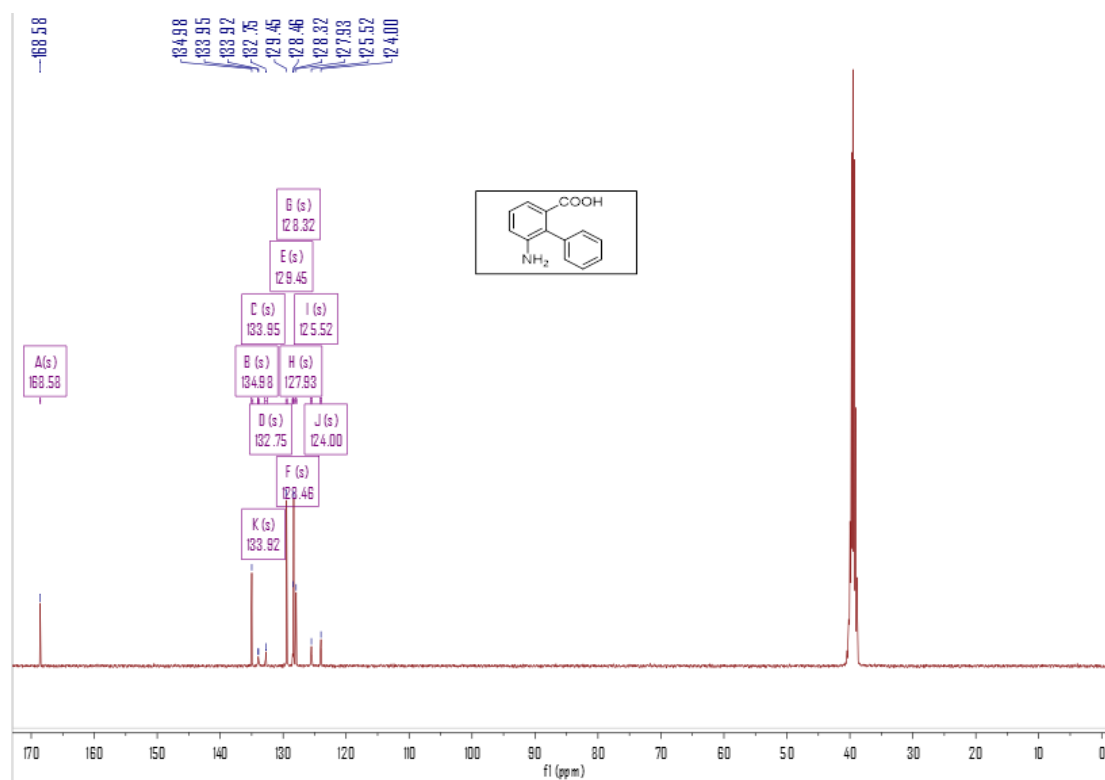


¹³C NMR spectra for **4q**.

6-amino-[1,1'-biphenyl]-2-carboxylic acid (4s)

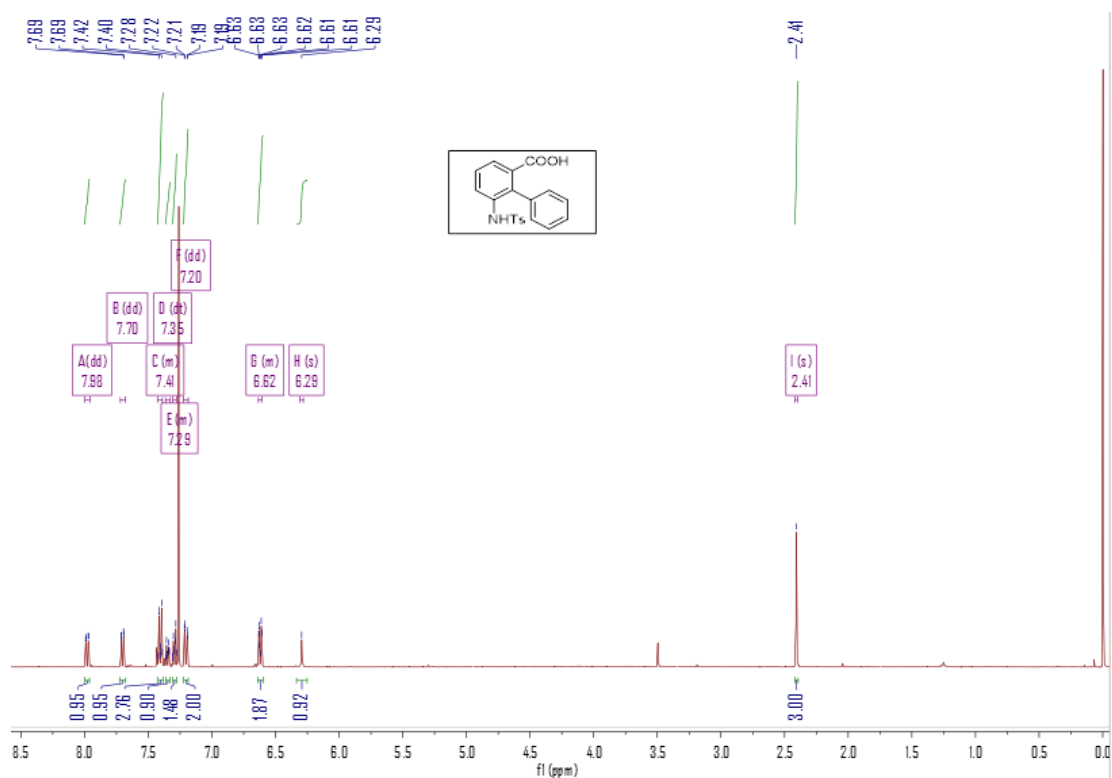


¹H NMR spectra for **4s**.

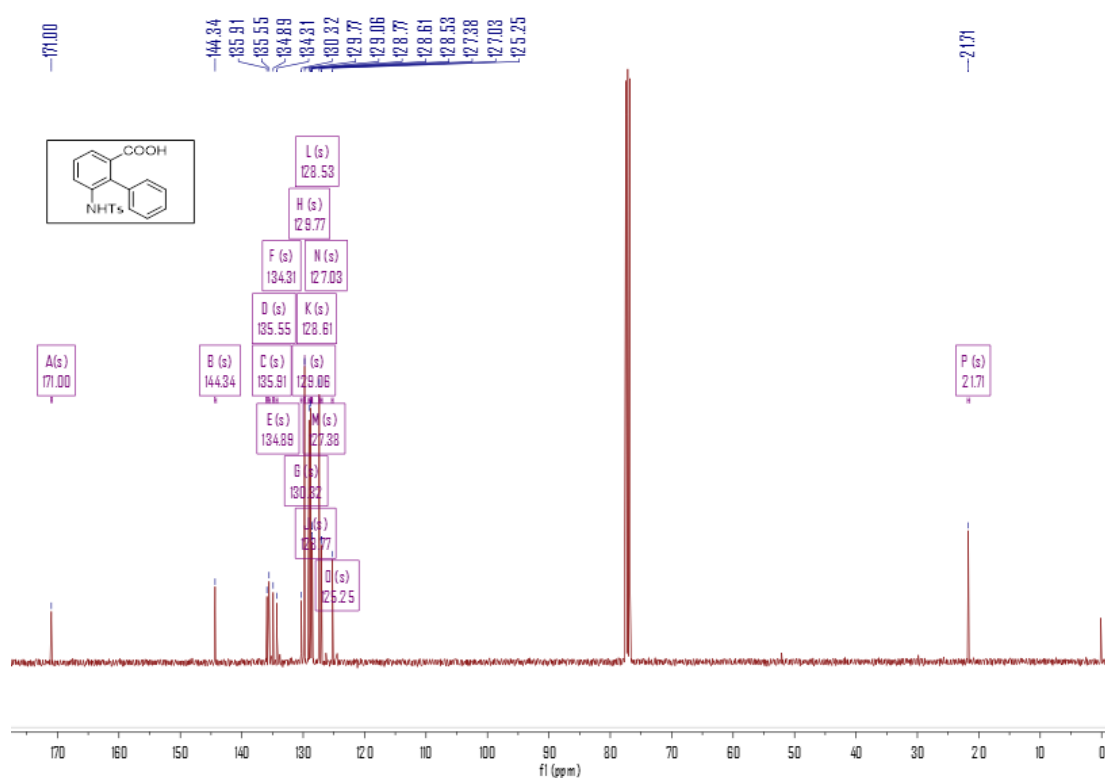


¹³C NMR spectra for **4s**.

6-((4-methylphenyl)sulfonamido)-[1,1'-biphenyl]-2-carboxylic acid (4t)

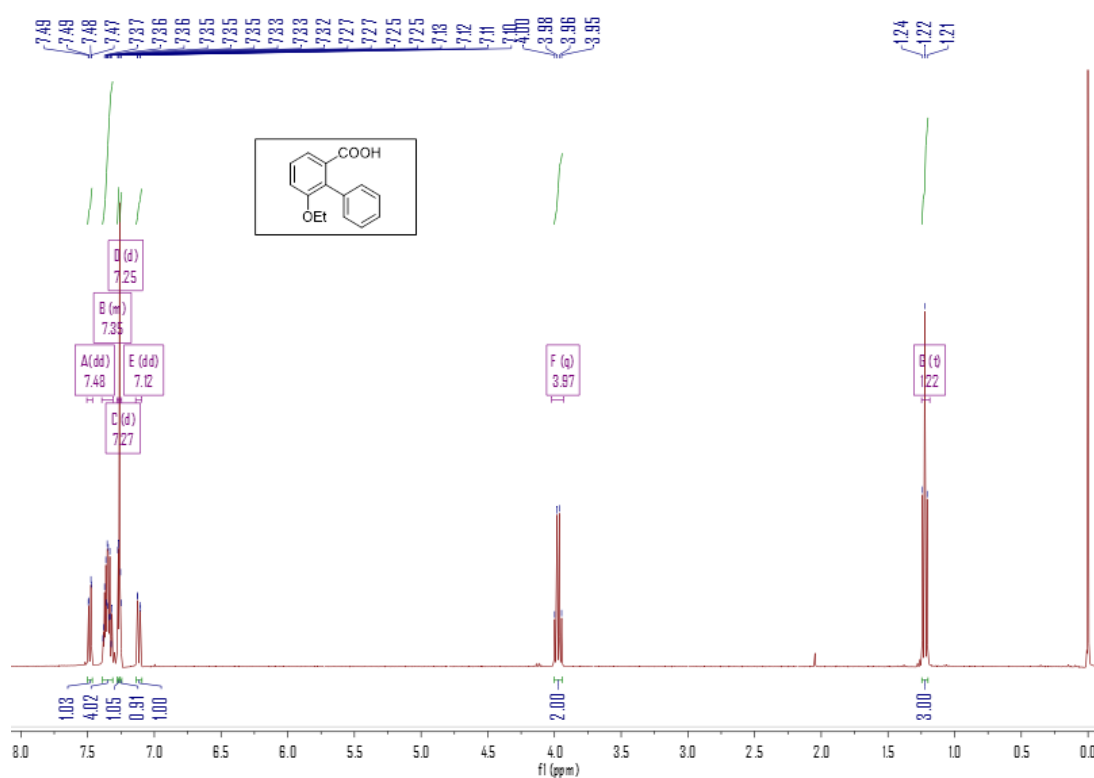


¹H NMR spectra for **4t**.

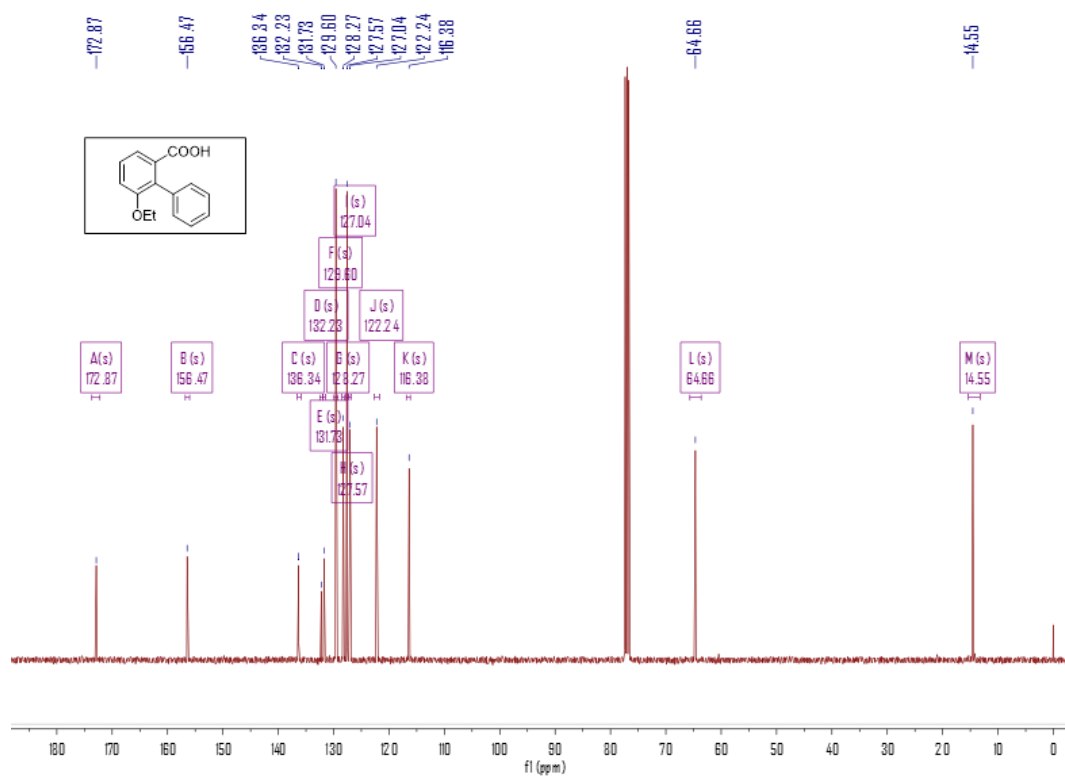


¹³C NMR spectra for **4t**.

6-ethoxy-[1,1'-biphenyl]-2-carboxylic acid (4u)

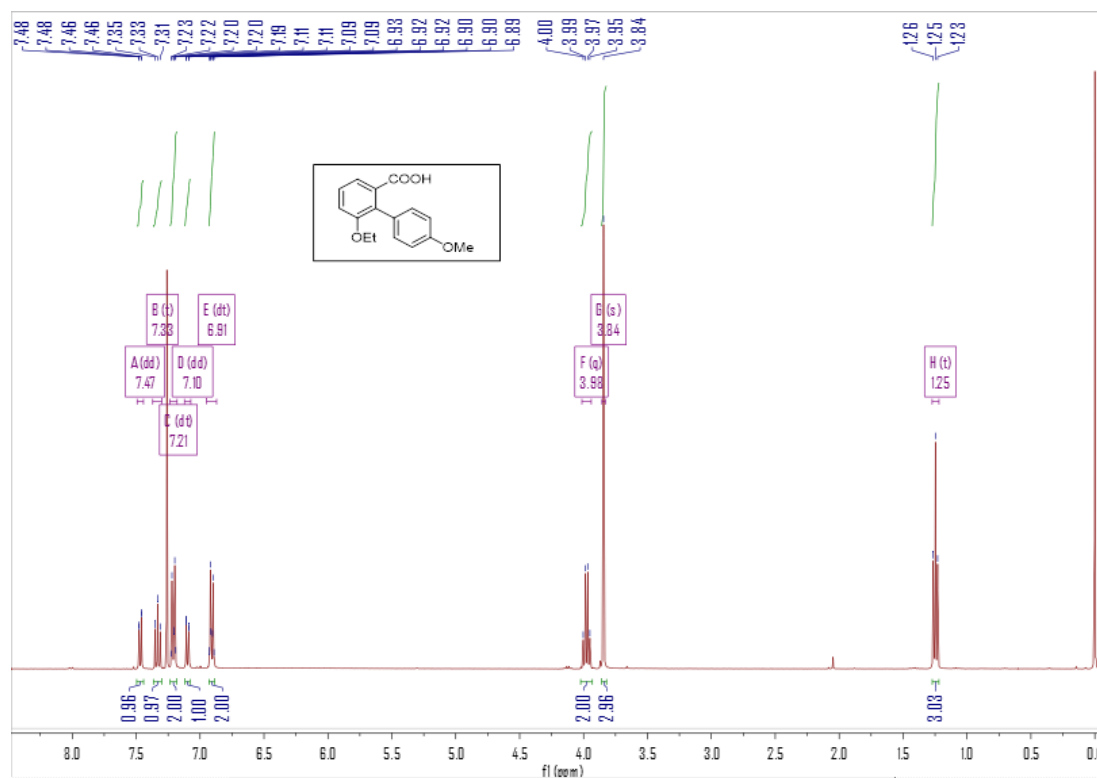


¹H NMR spectra for **4u**.

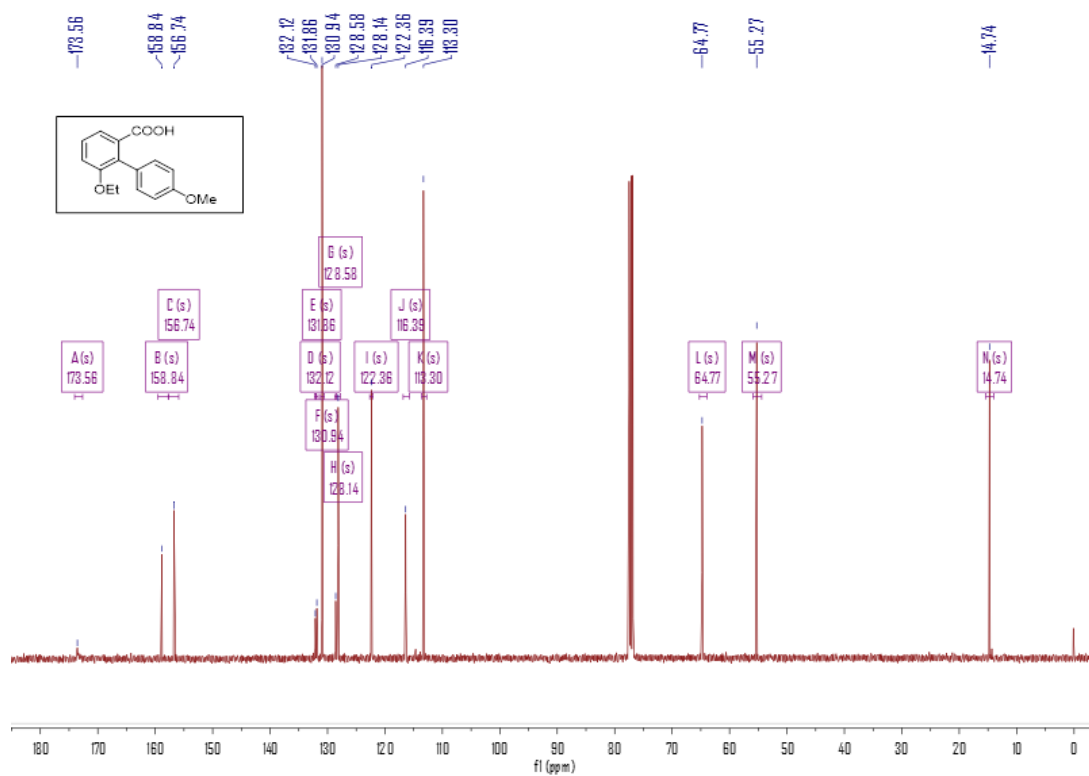


¹³C NMR spectra for **4u**.

6-ethoxy-4'-methoxy-[1,1'-biphenyl]-2-carboxylic acid (4v)

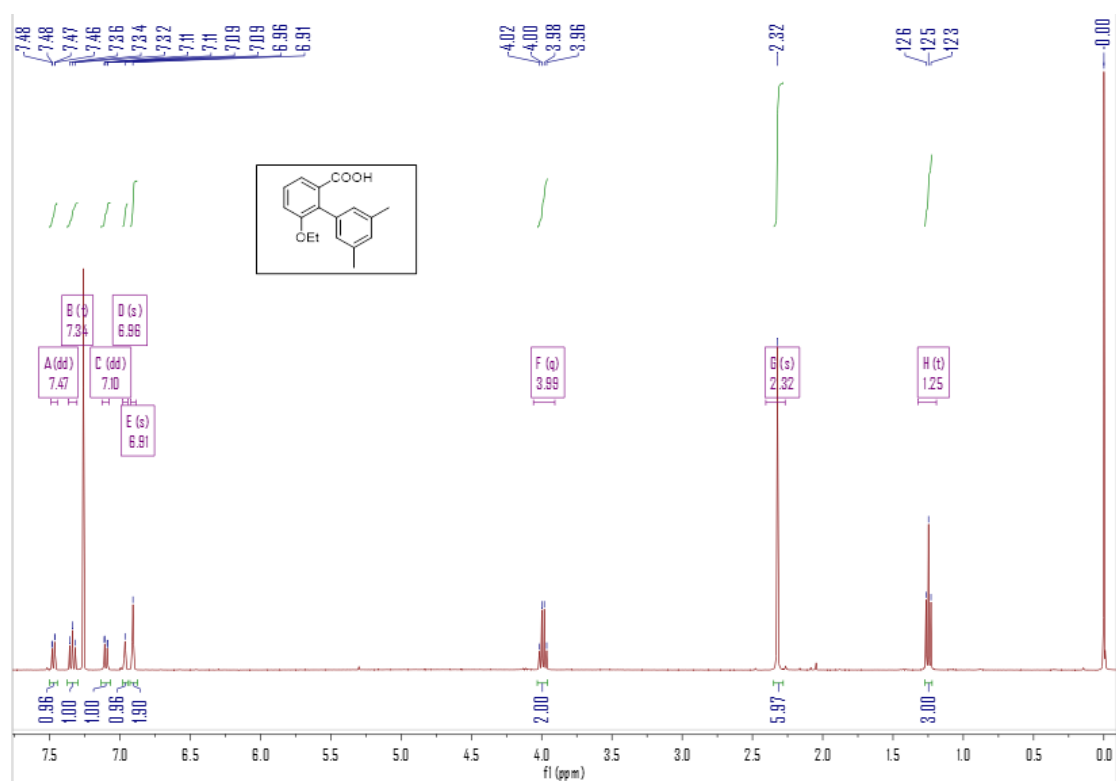


¹H NMR spectra for **4v**.

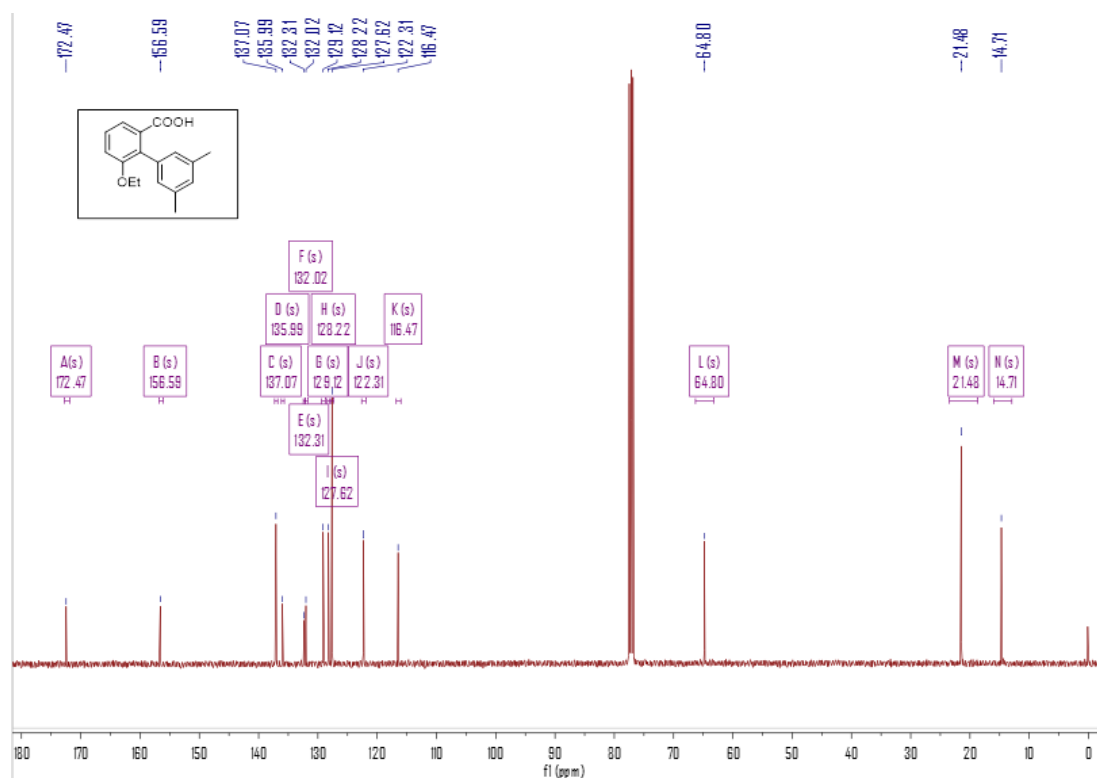


¹³C NMR spectra for **4v**.

6-ethoxy-3',5'-dimethyl-[1,1'-biphenyl]-2-carboxylic acid (4w)

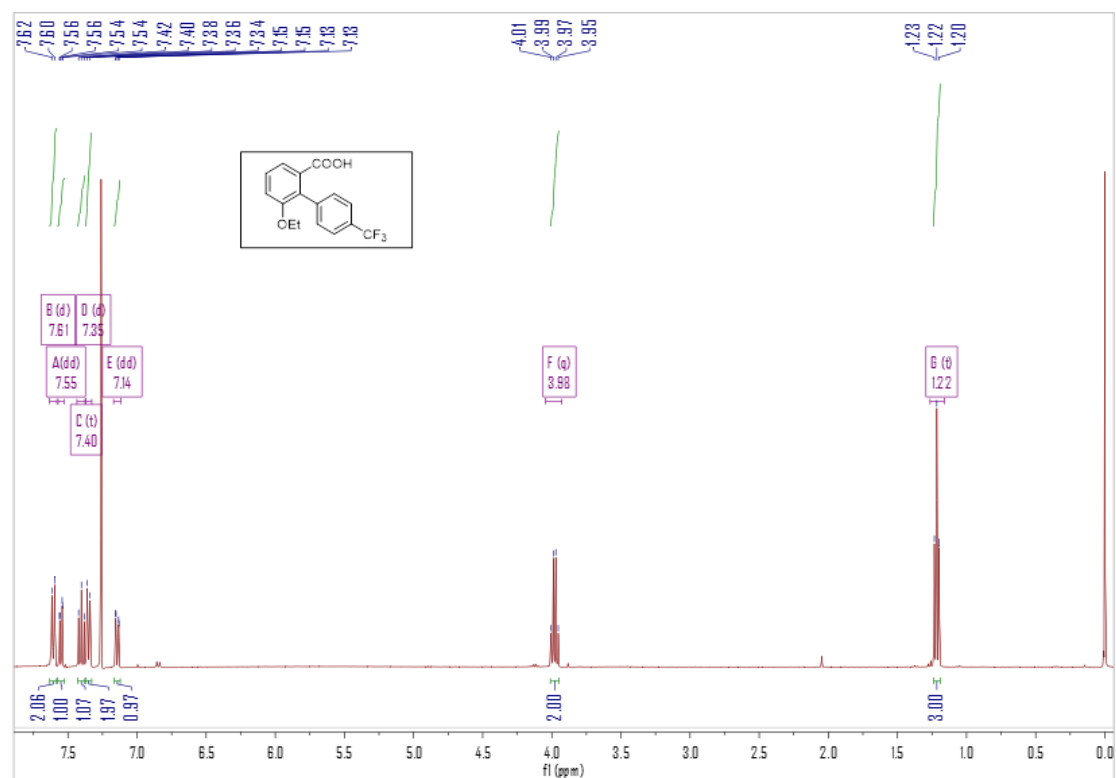


¹H NMR spectra for **4w**.

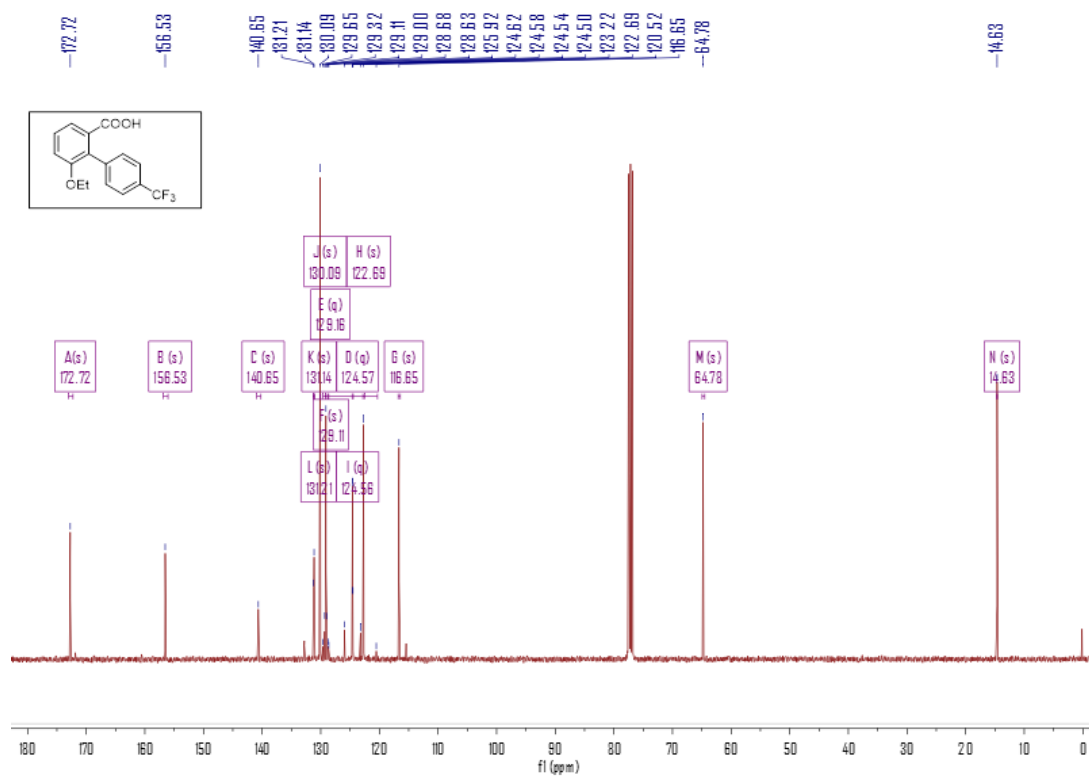


¹³C NMR spectra for **4w**.

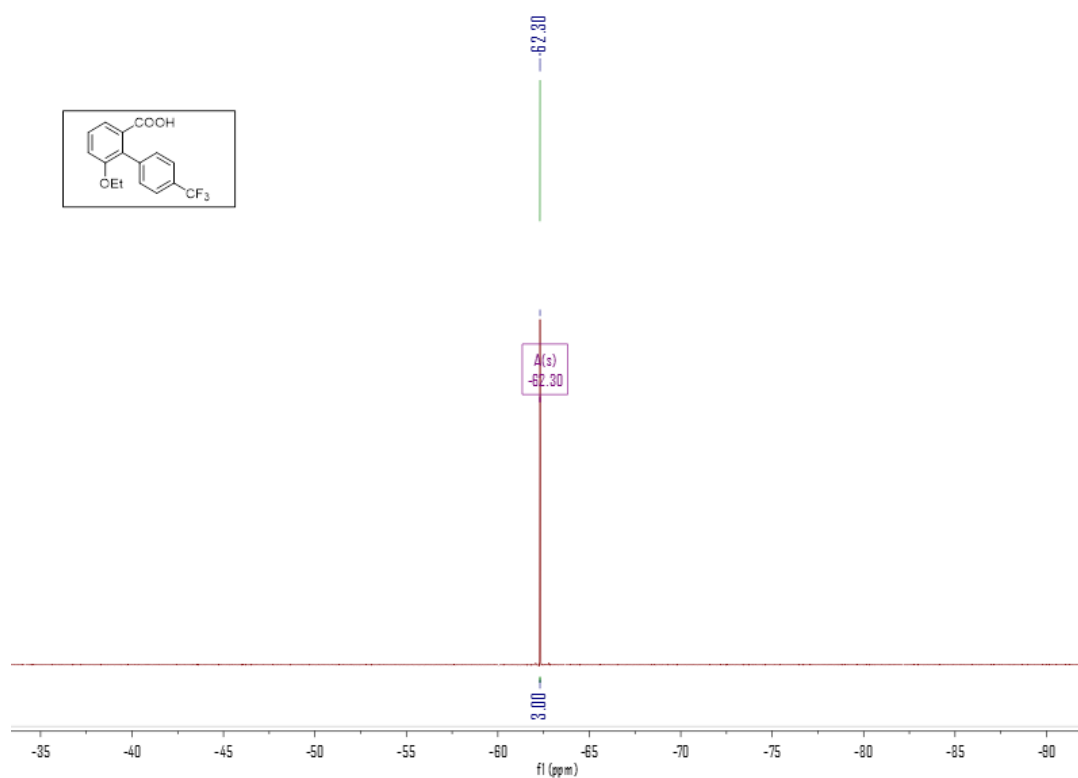
6-ethoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid (4x**)**



¹H NMR spectra for **4x**.

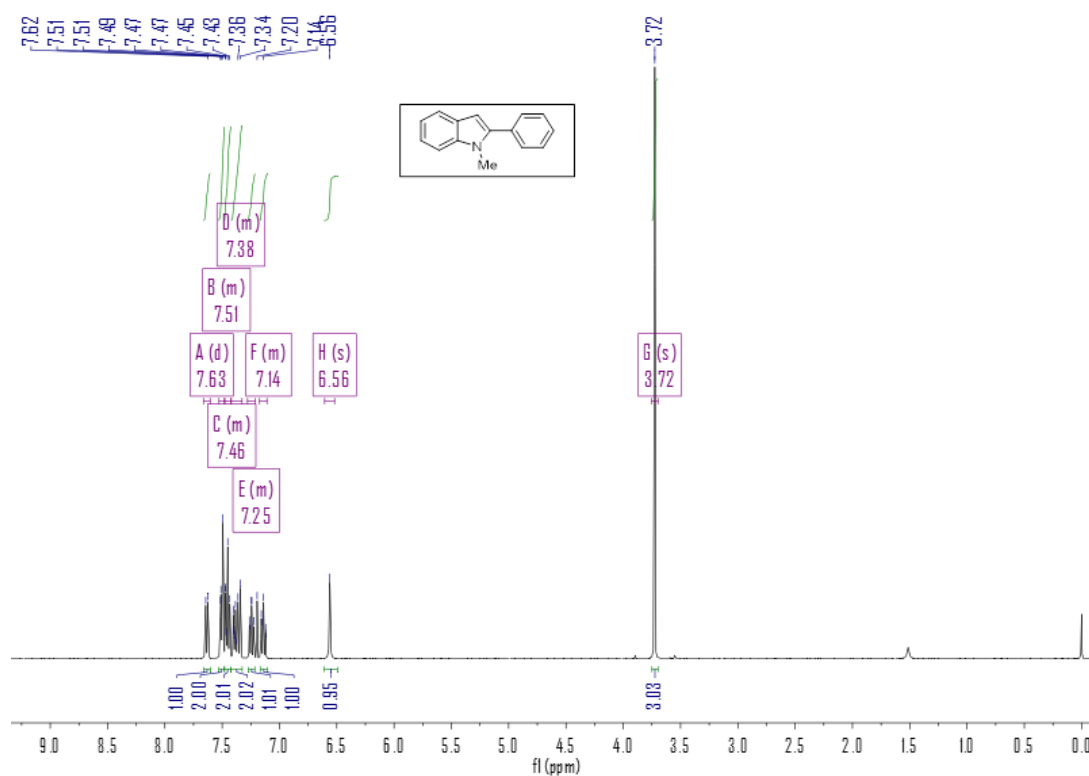


¹³C NMR spectra for 4x.

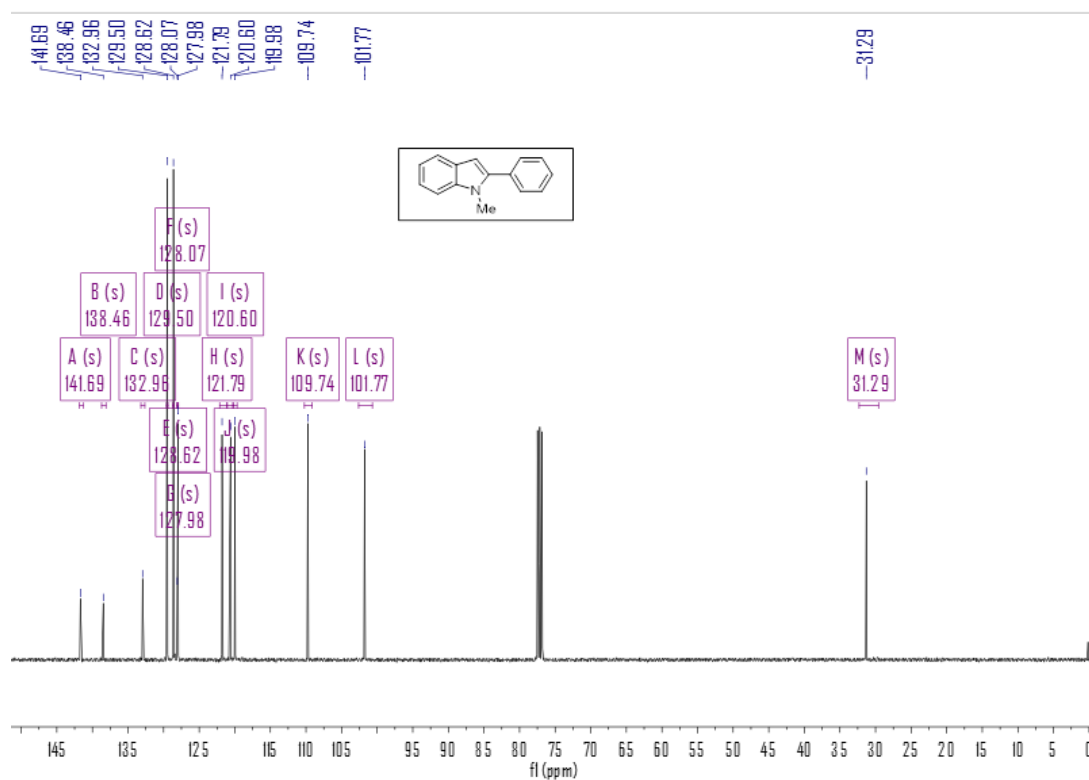


¹⁹F NMR spectra for 4x.

1-methyl-2-phenyl-indole (3b)

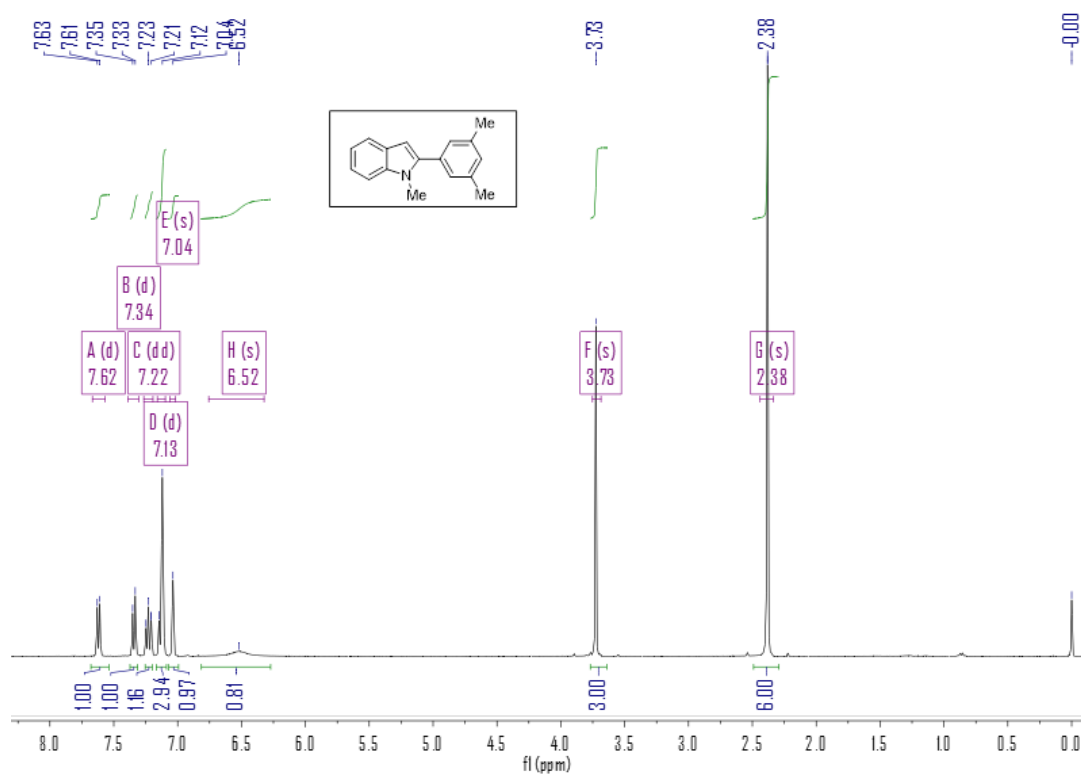


¹H NMR spectra for **3b**.

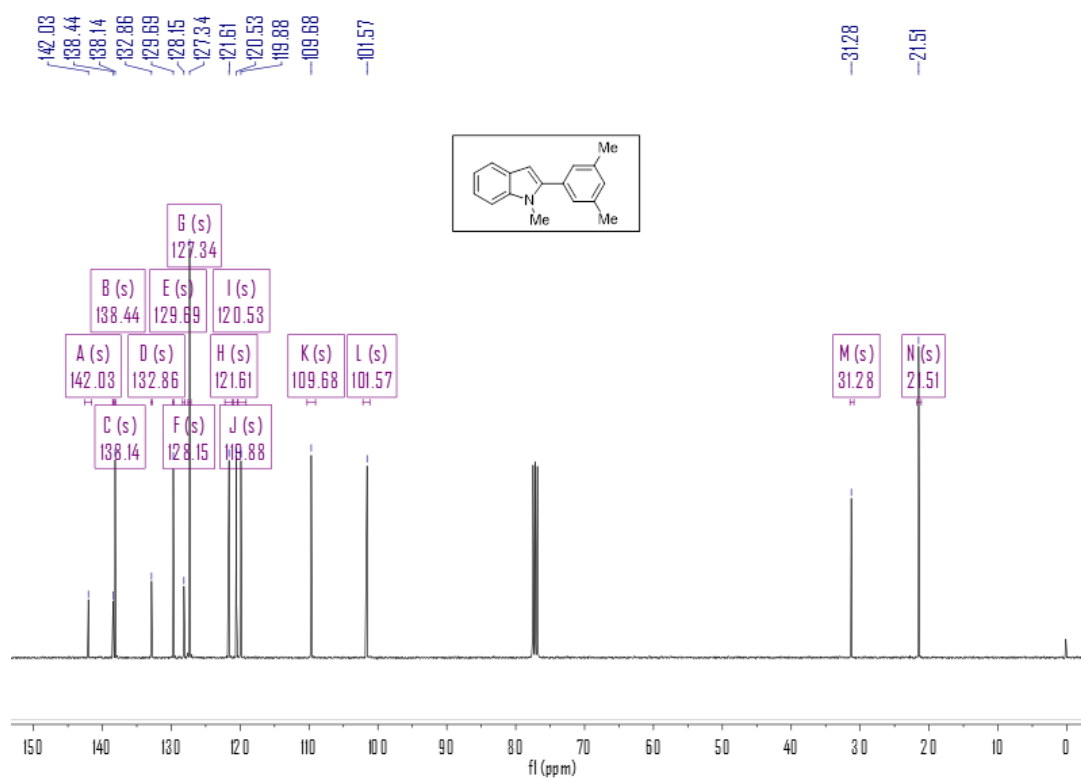


¹³C NMR spectra for **3b**.

2-(3,5-dimethylphenyl)-1-methylindole (3d)

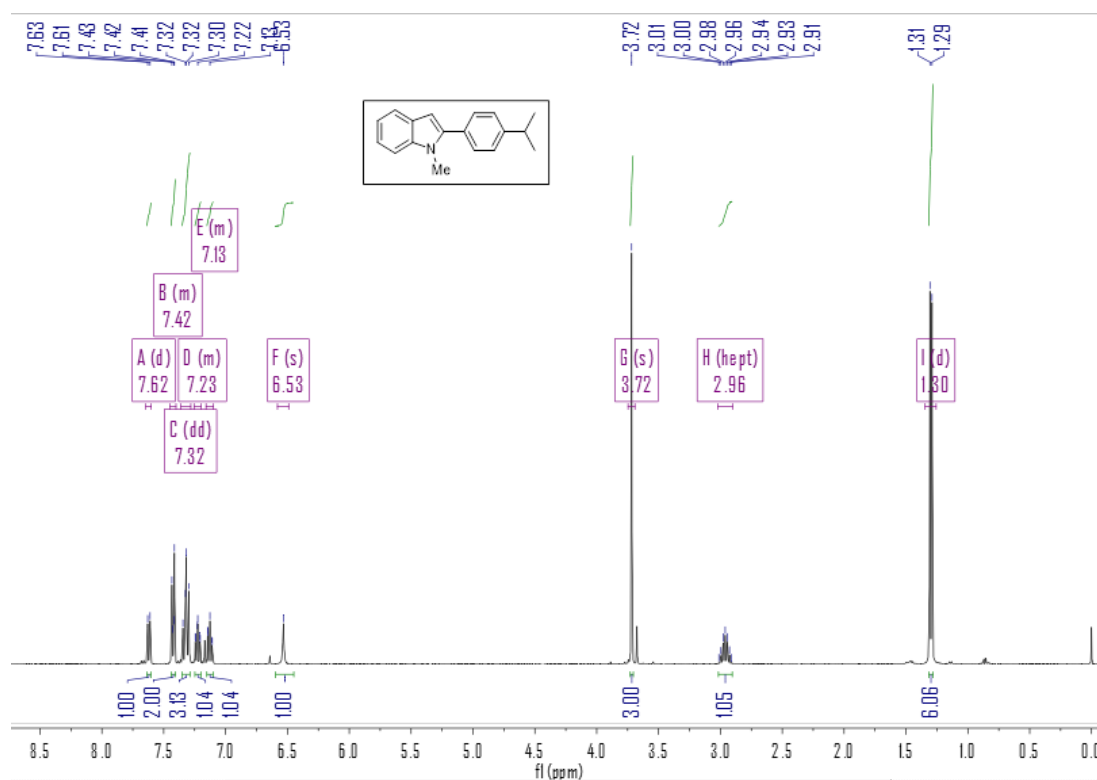


¹H NMR spectra for **3d**.

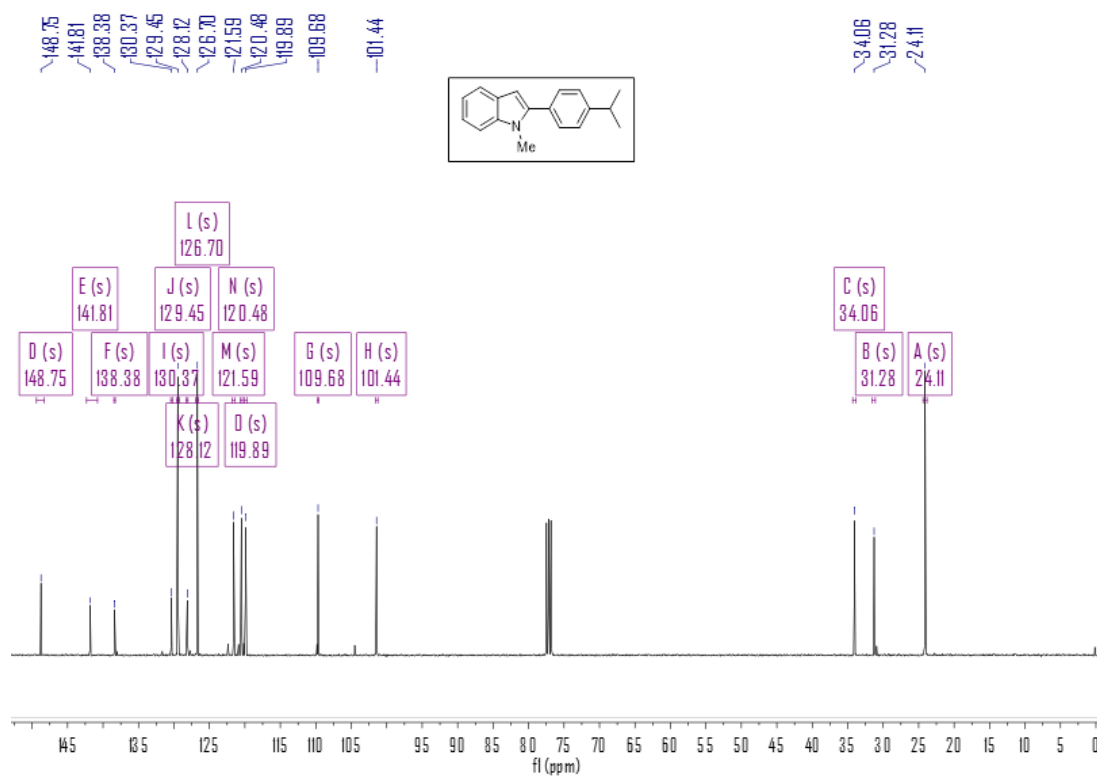


¹³C NMR spectra for **3d**.

2-(4-isopropylphenyl)-1-methylindole (**3e**)

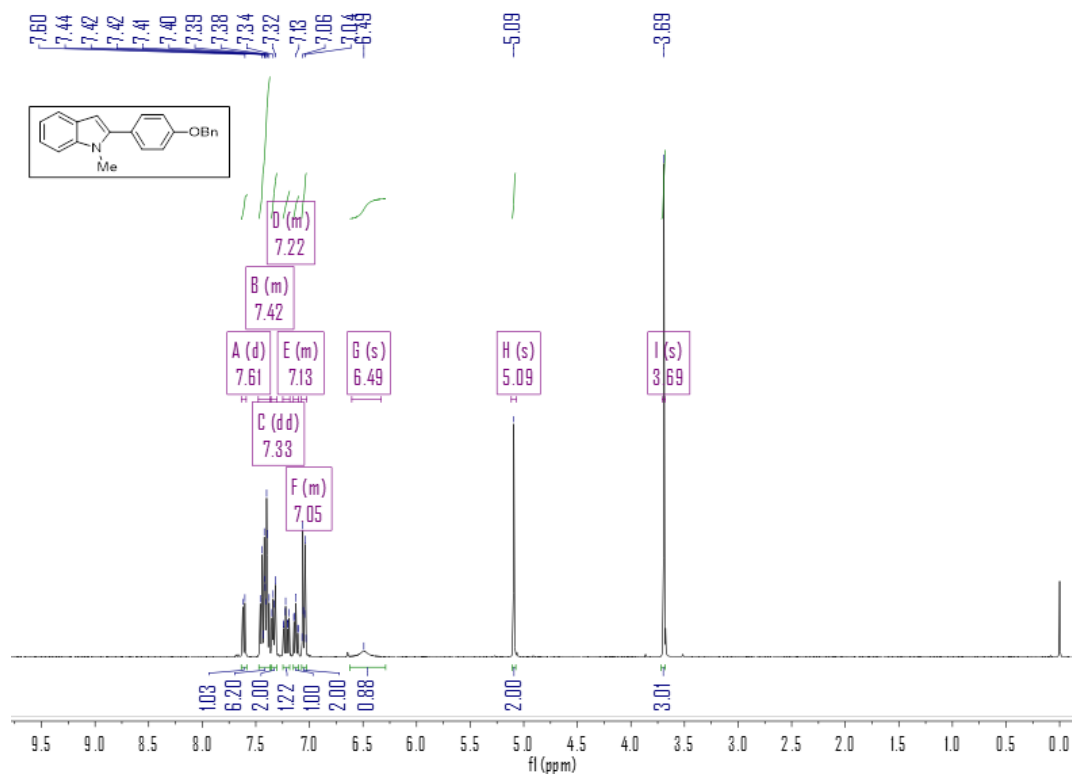


¹H NMR spectra for 3e.

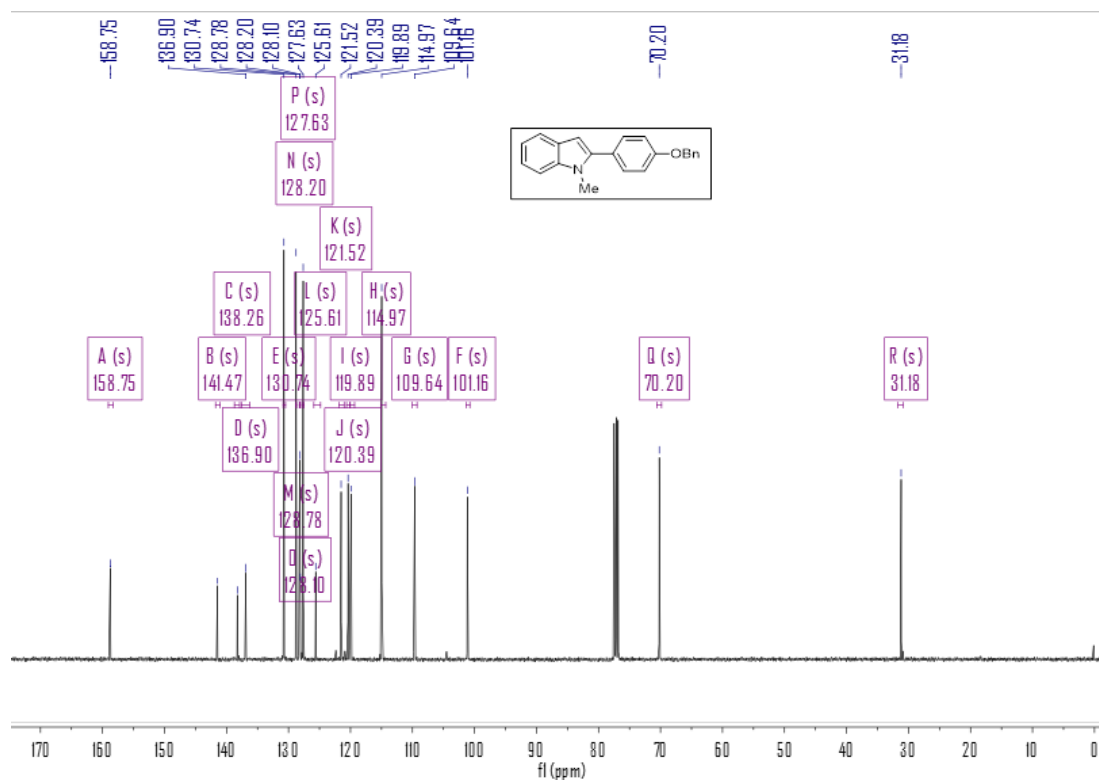


¹³C NMR spectra for 3e.

2-(4-(benzyloxy)phenyl)-1-methylindole (3f)

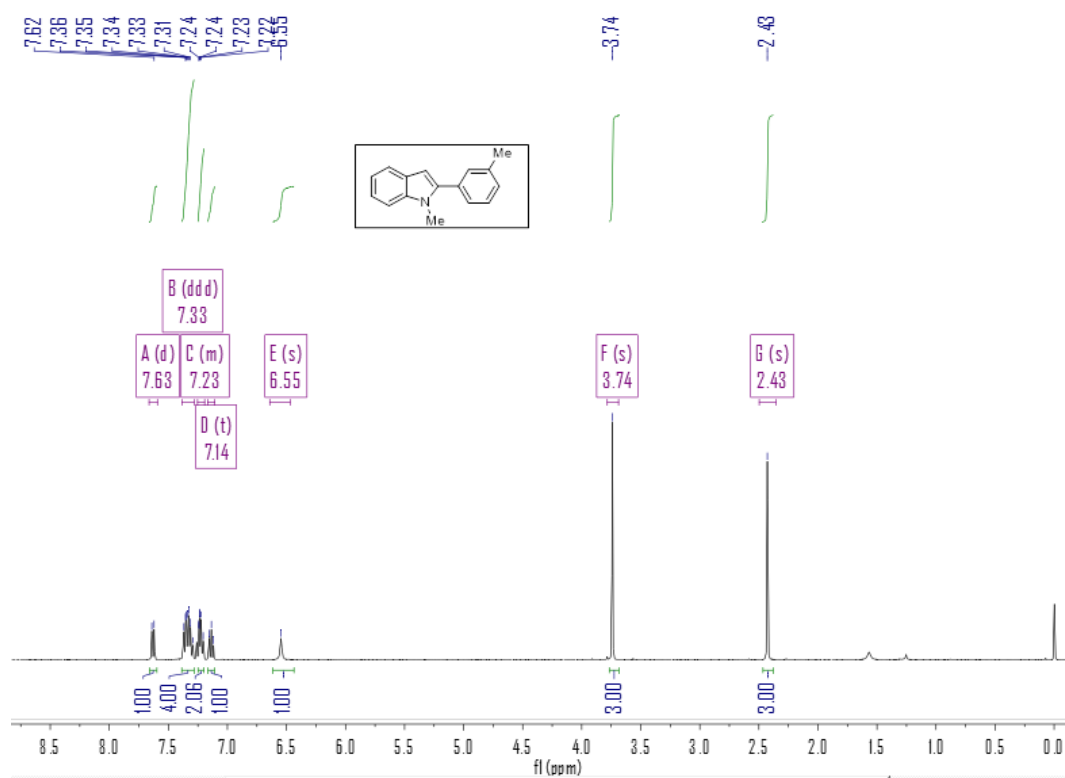


¹H NMR spectra for 3f.

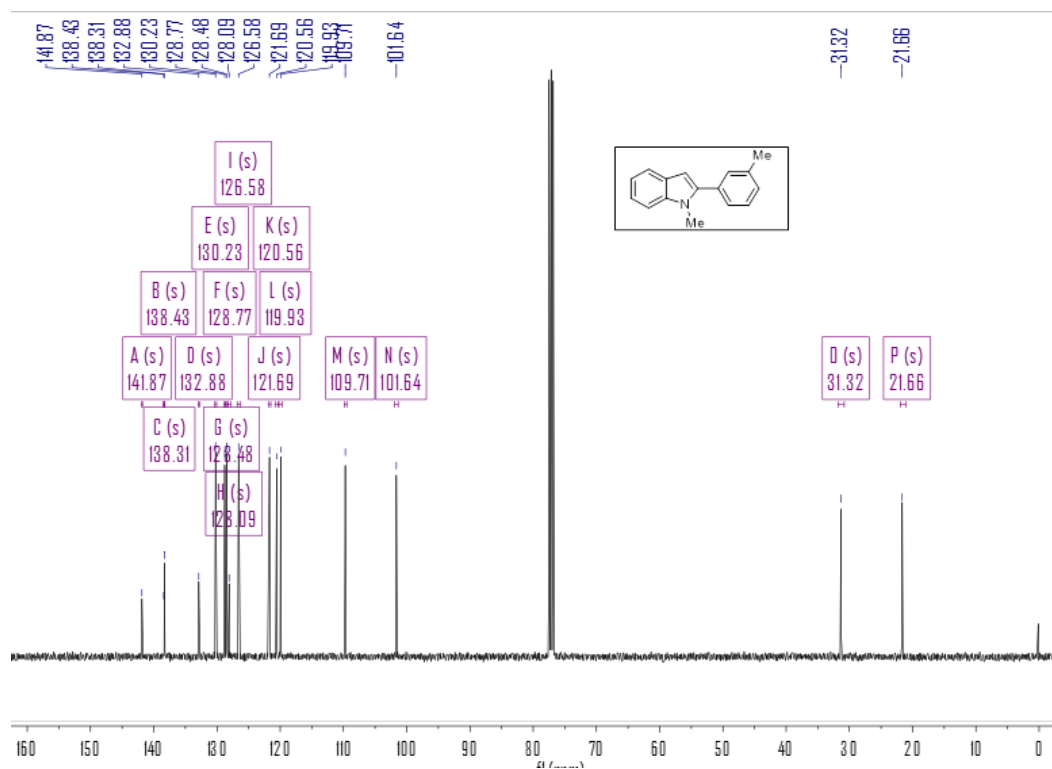


¹³C NMR spectra for 3f.

1-methyl-2-(m-tolyl)-indole (3g)

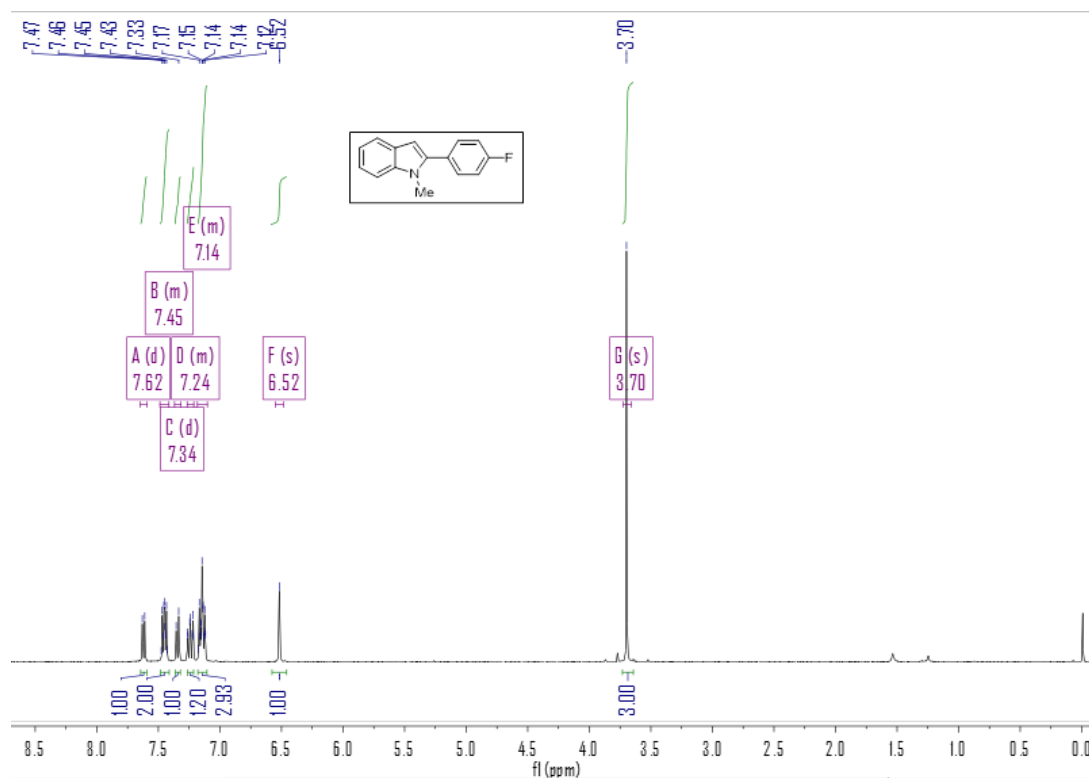


¹H NMR spectra for **3g**.

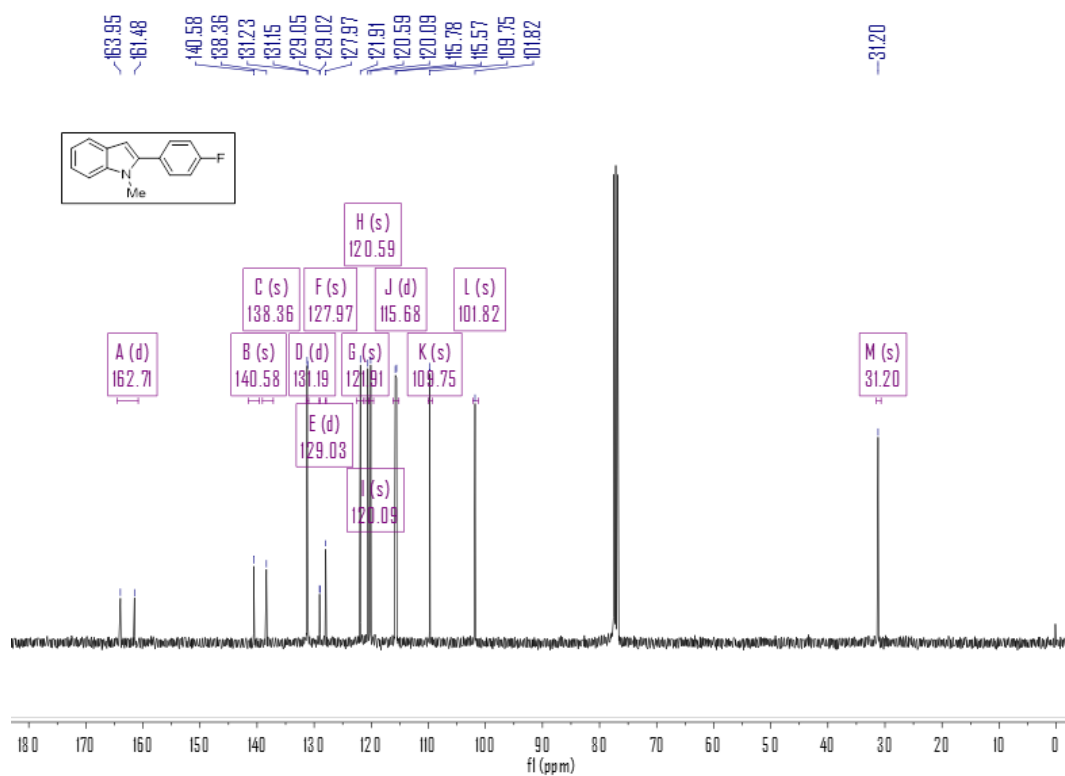


¹³C NMR spectra for **3g**

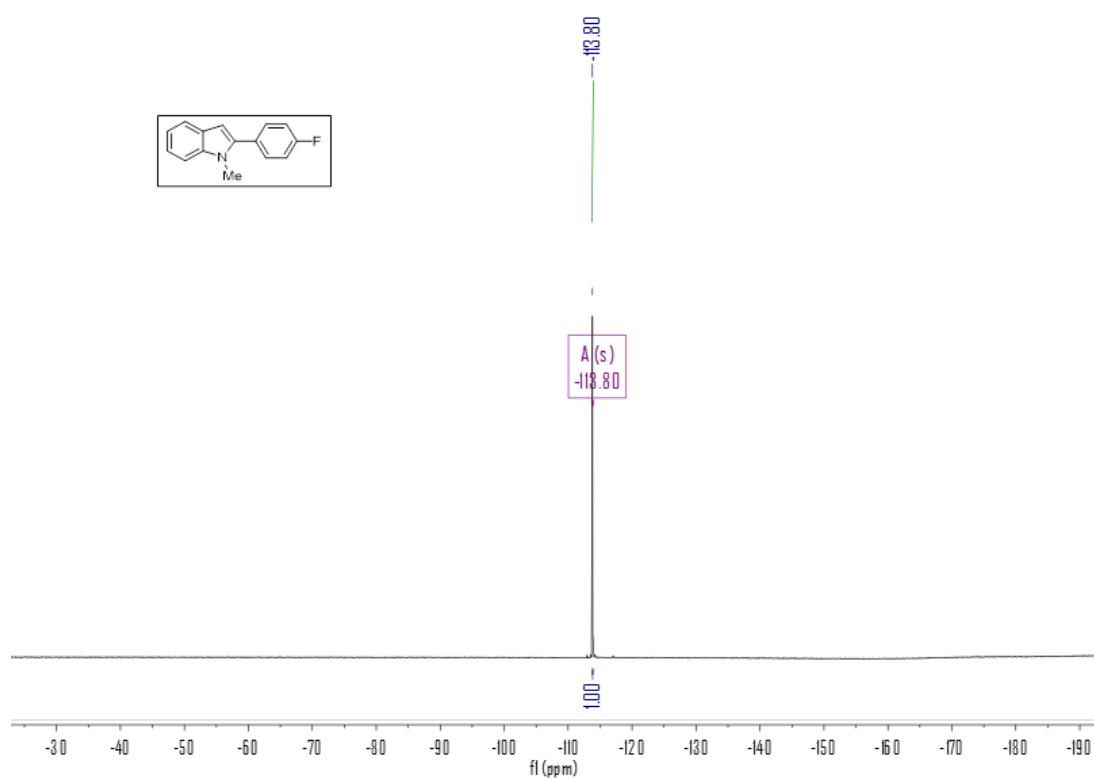
2-(4-fluorophenyl)-1-methylindole (**3h**)



^1H NMR spectra for **3h**.

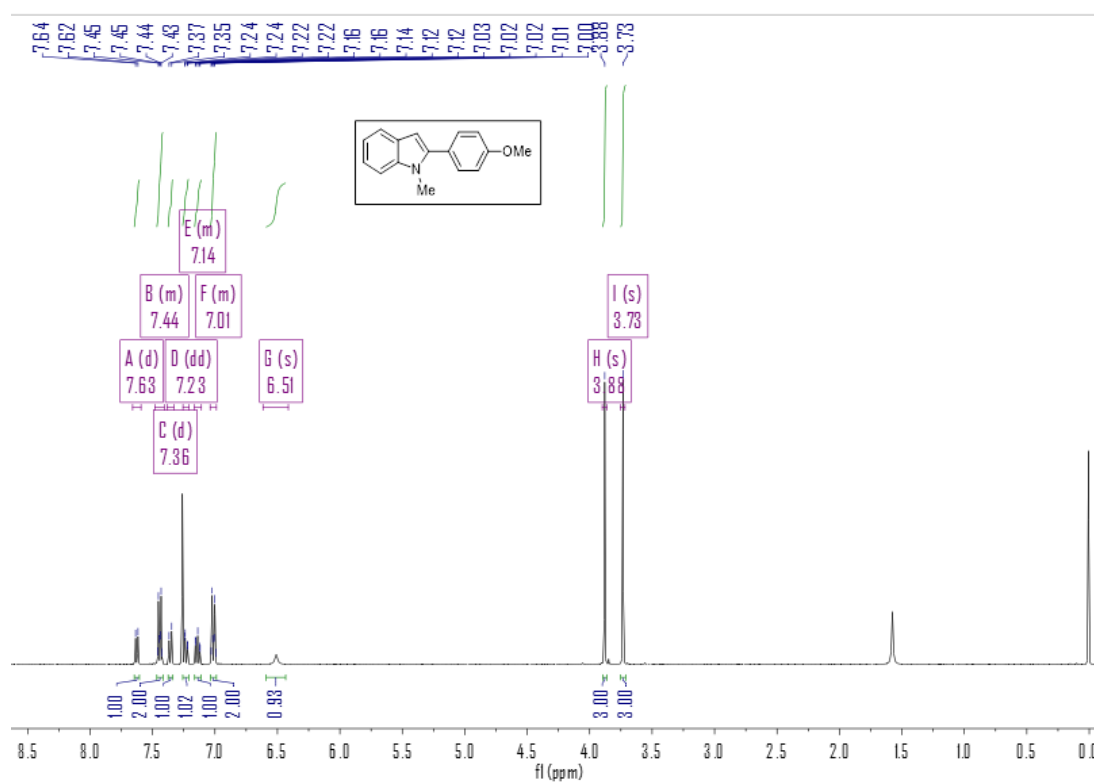


^{13}C NMR spectra for **3h**.

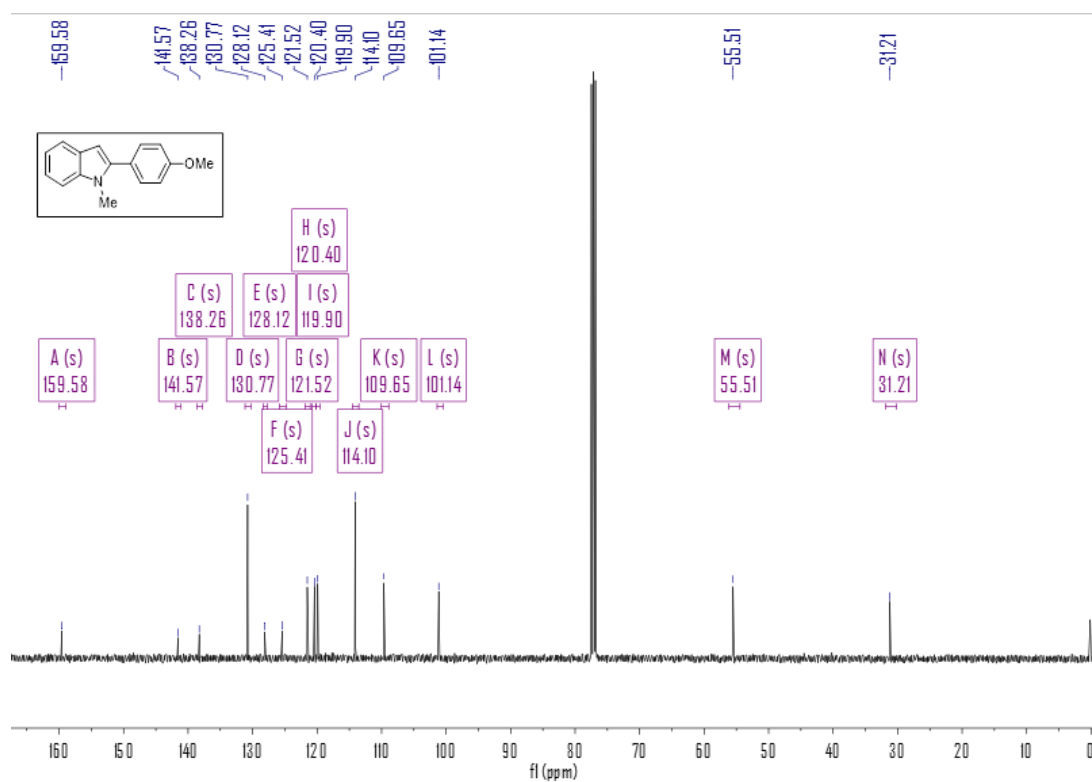


^{19}F NMR spectra for 3h.

2-(4-methoxyphenyl)-1-methylindole (3i)

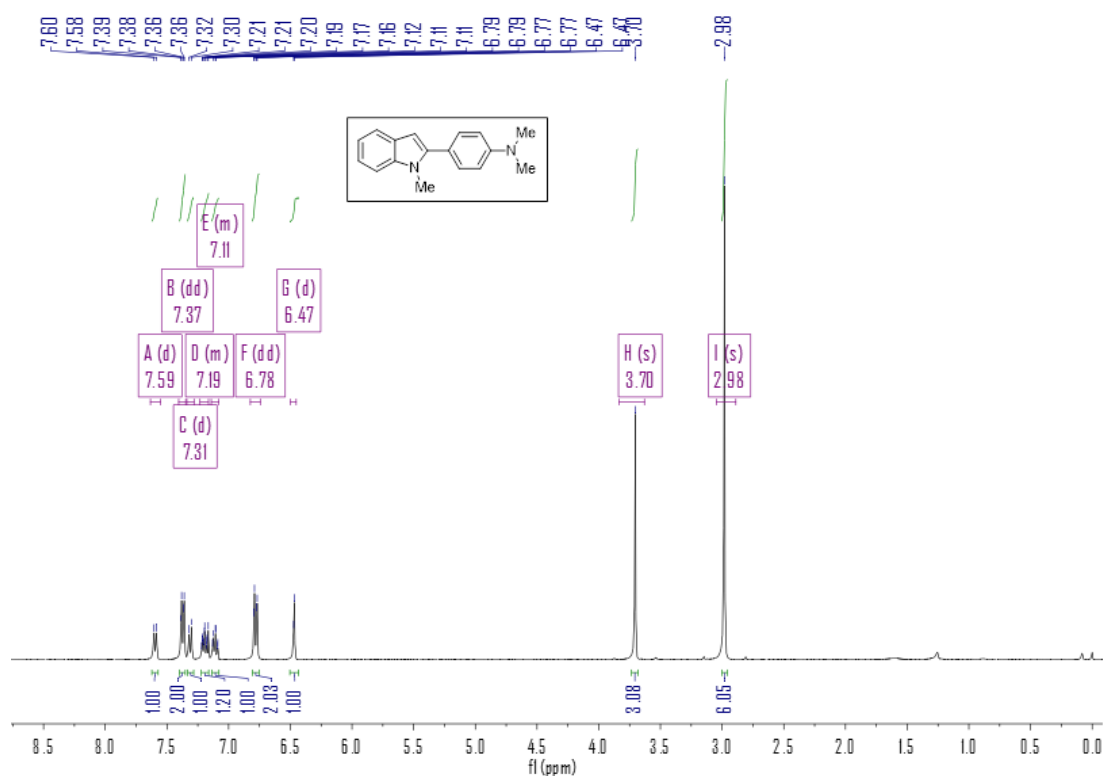


^1H NMR spectra for 3i.

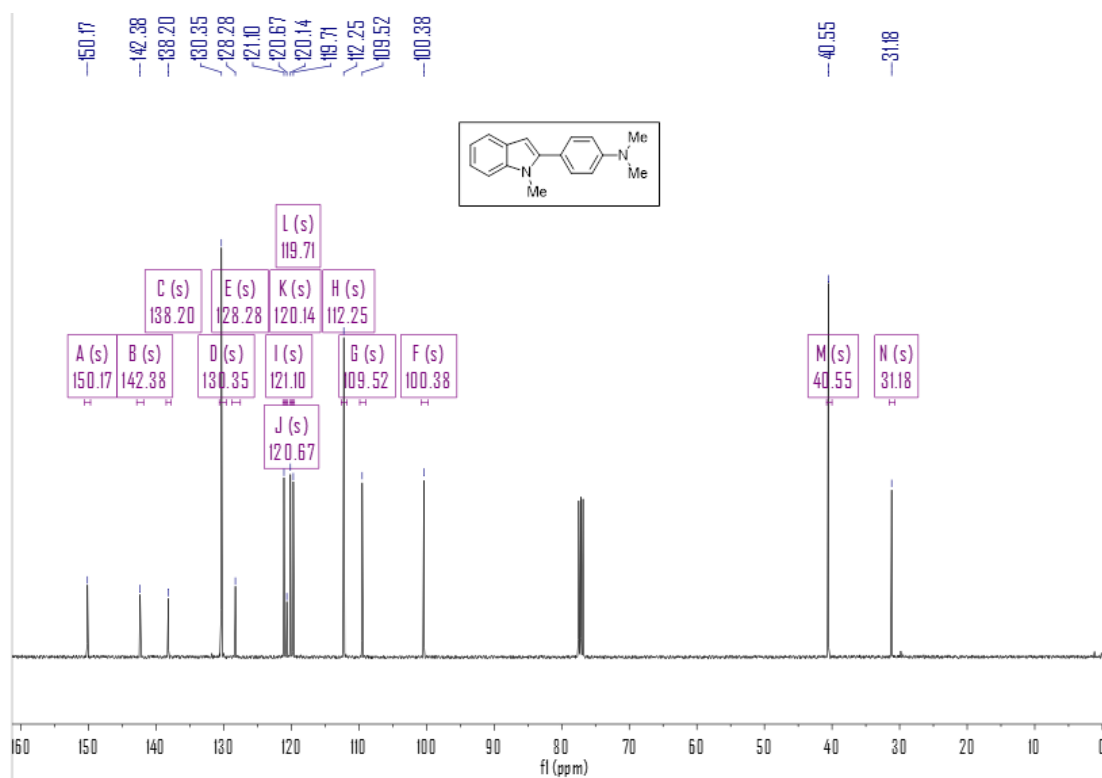


¹³C NMR spectra for **3i**.

***N,N*-dimethyl-4-(1-methylindol-2-yl)aniline (**3j**)**

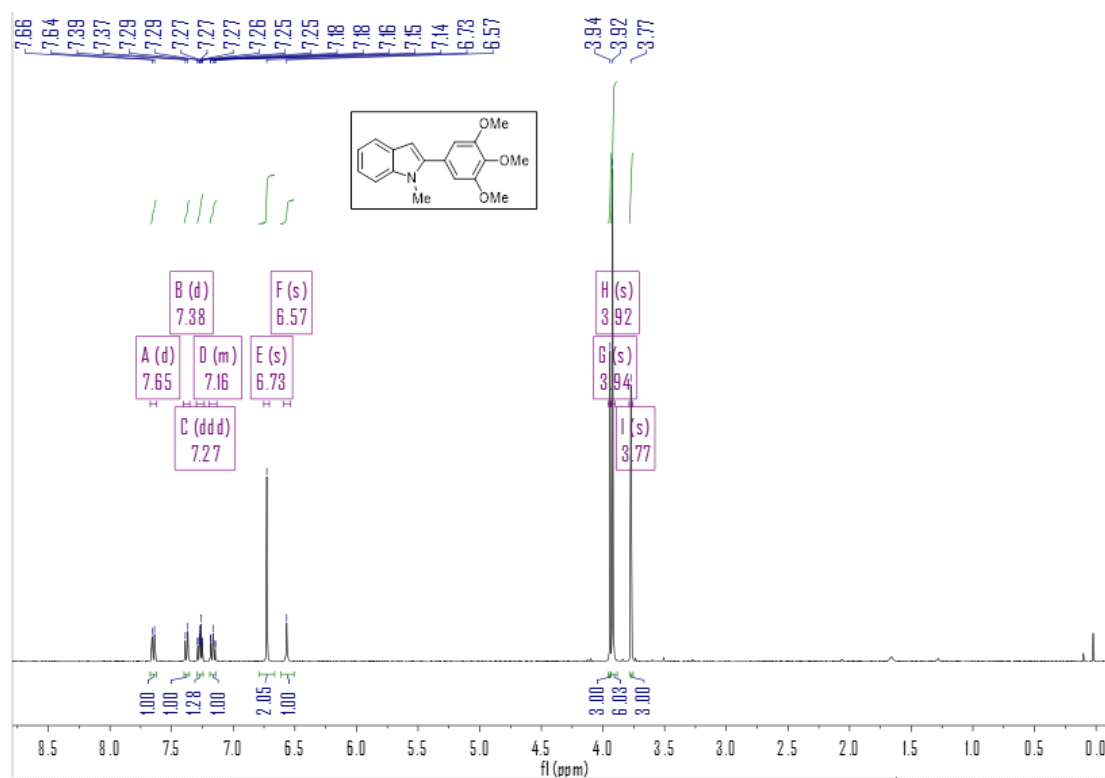


¹H NMR spectra for **3j**.

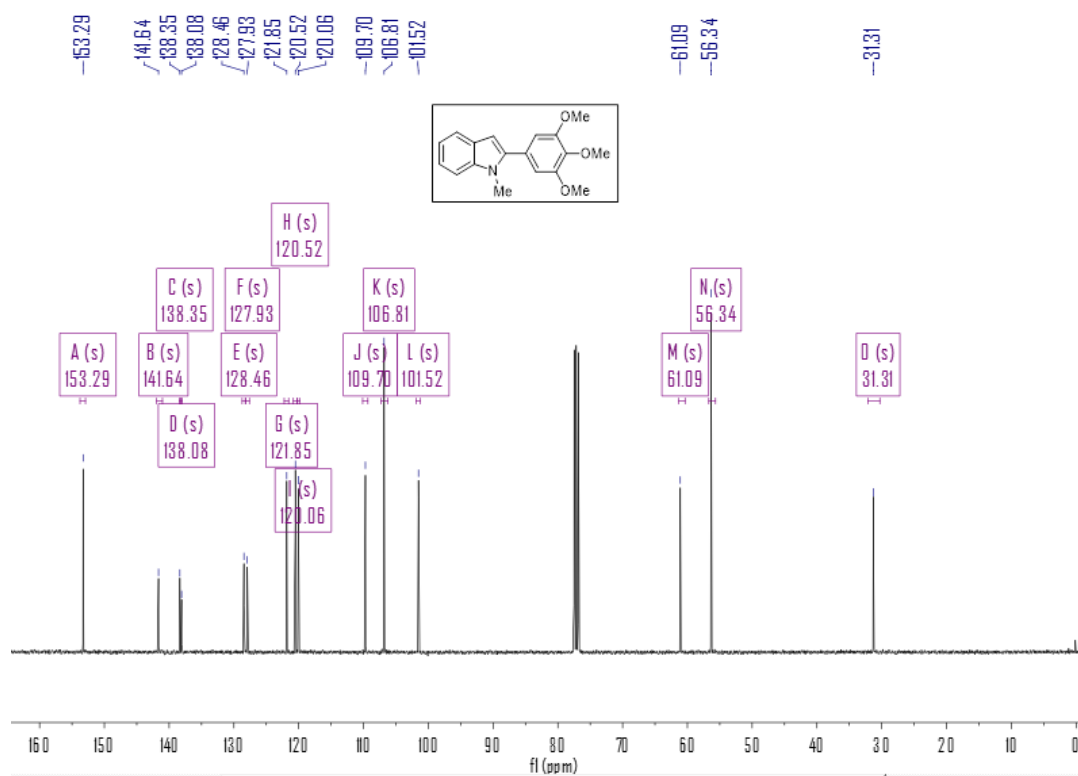


¹³C NMR spectra for **3j**.

1-methyl-2-(3,4,5-trimethoxyphenyl)-indole (3k)

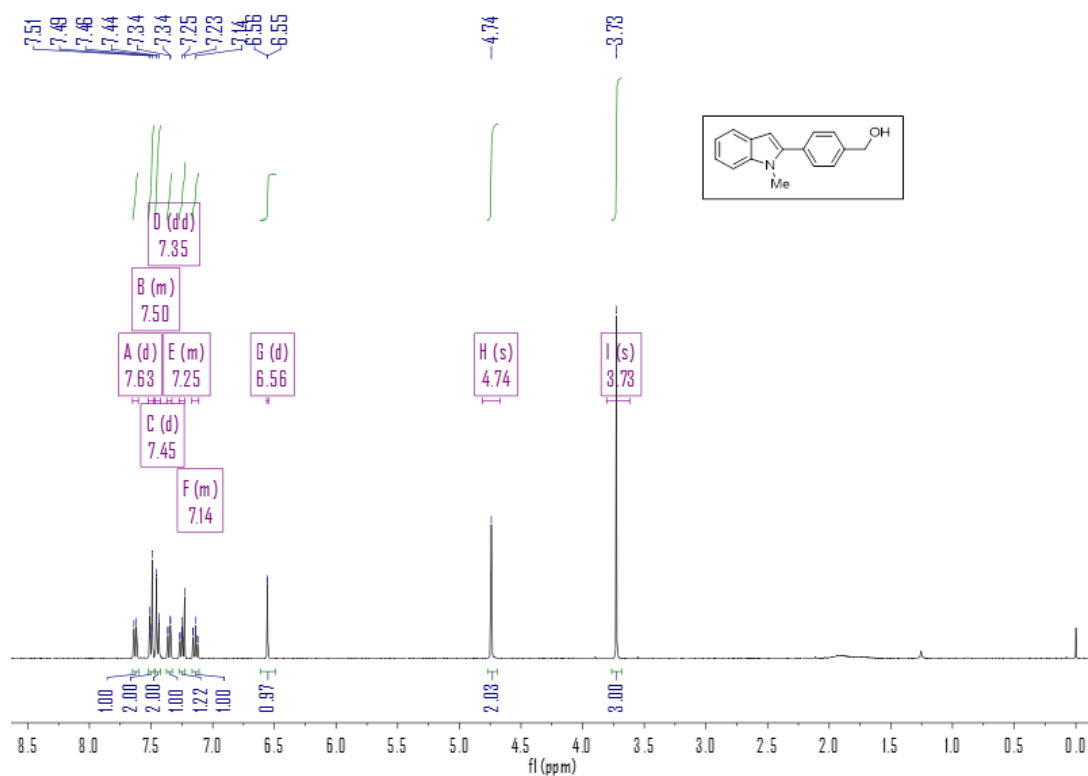


¹H NMR spectra for **3k**.

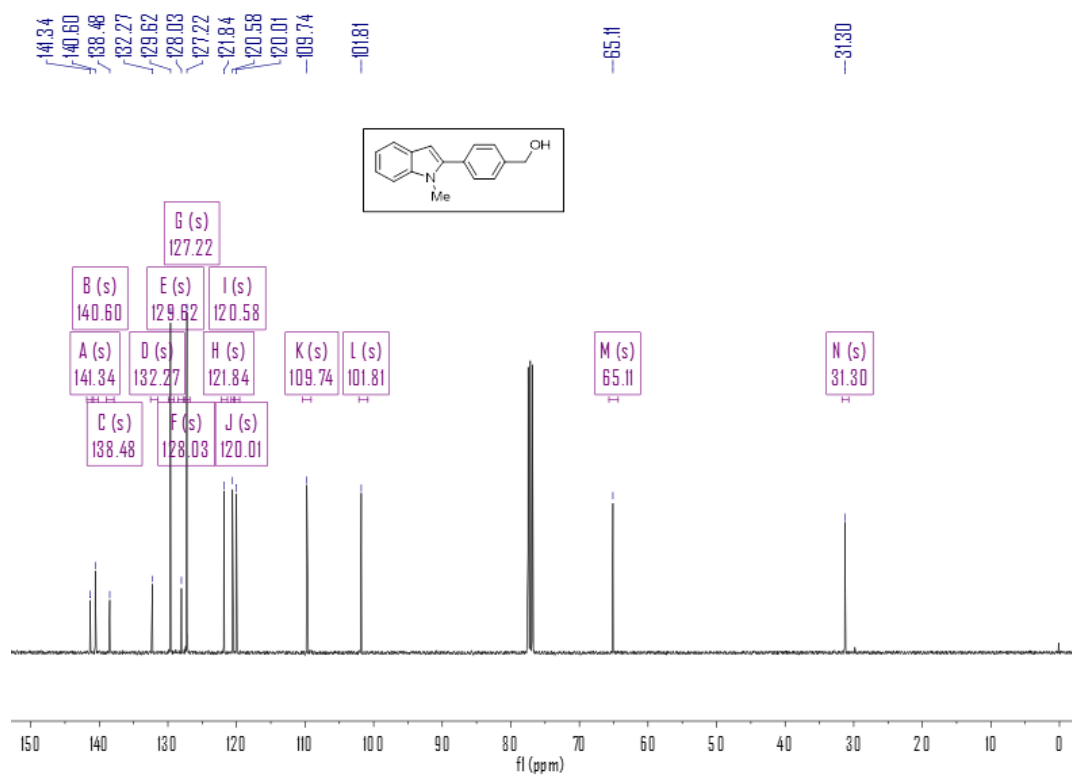


¹³C NMR spectra for **3l**.

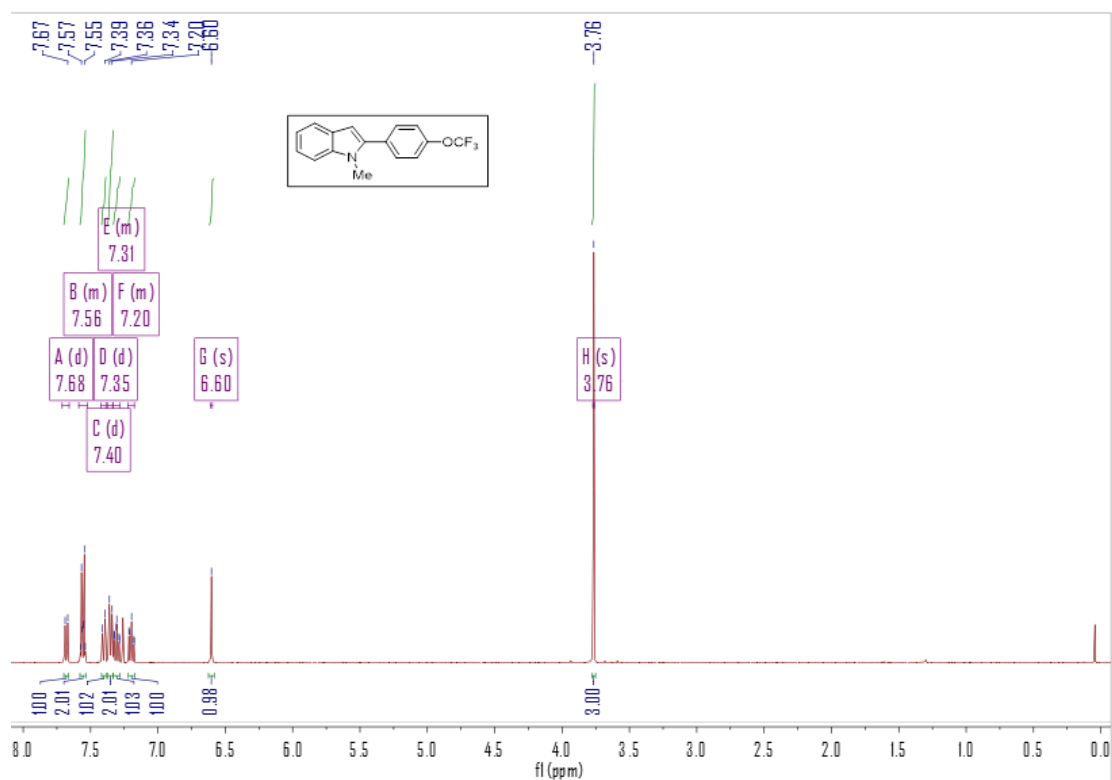
(4-(1-methylindol-2-yl)phenyl)methanol (3l)



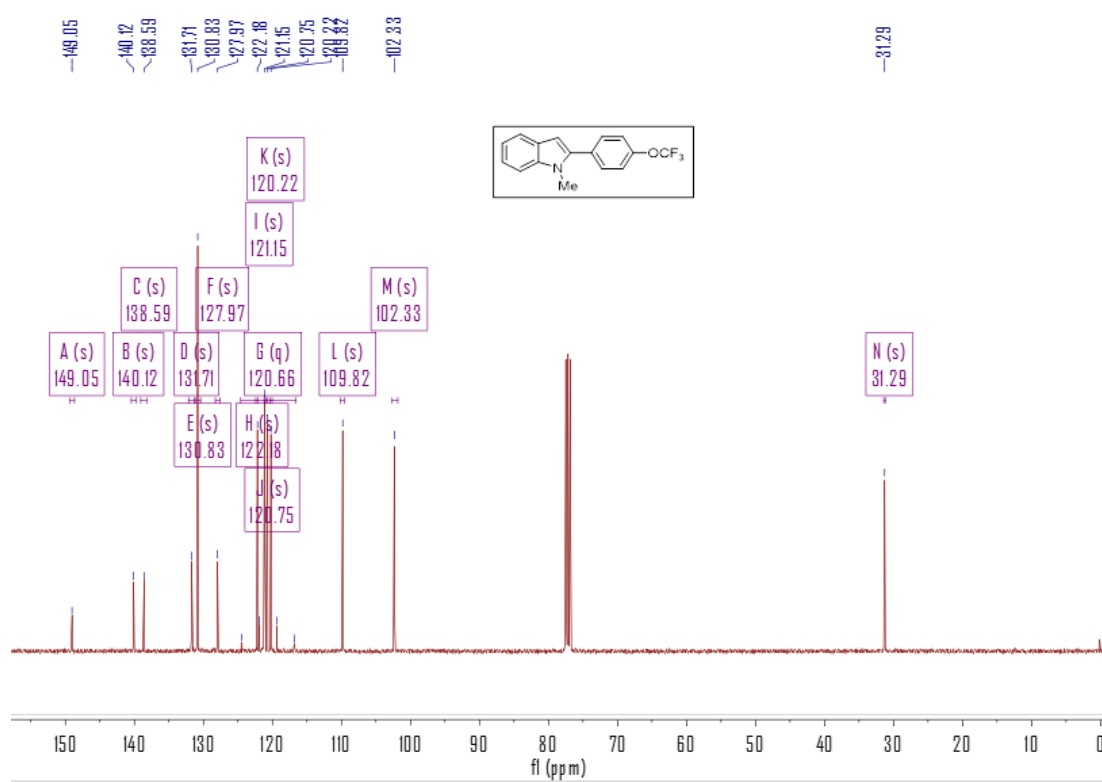
¹H NMR spectra for **3l**.



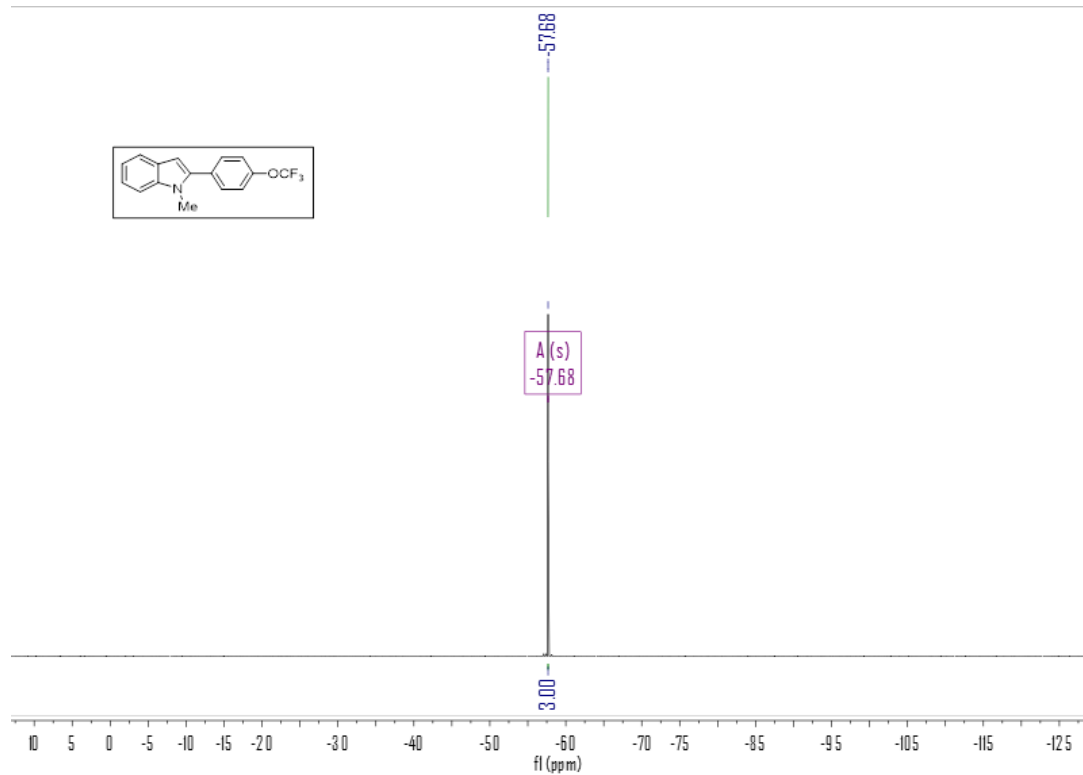
¹³C NMR spectra for **3l**.



¹H NMR spectra for **3m**.

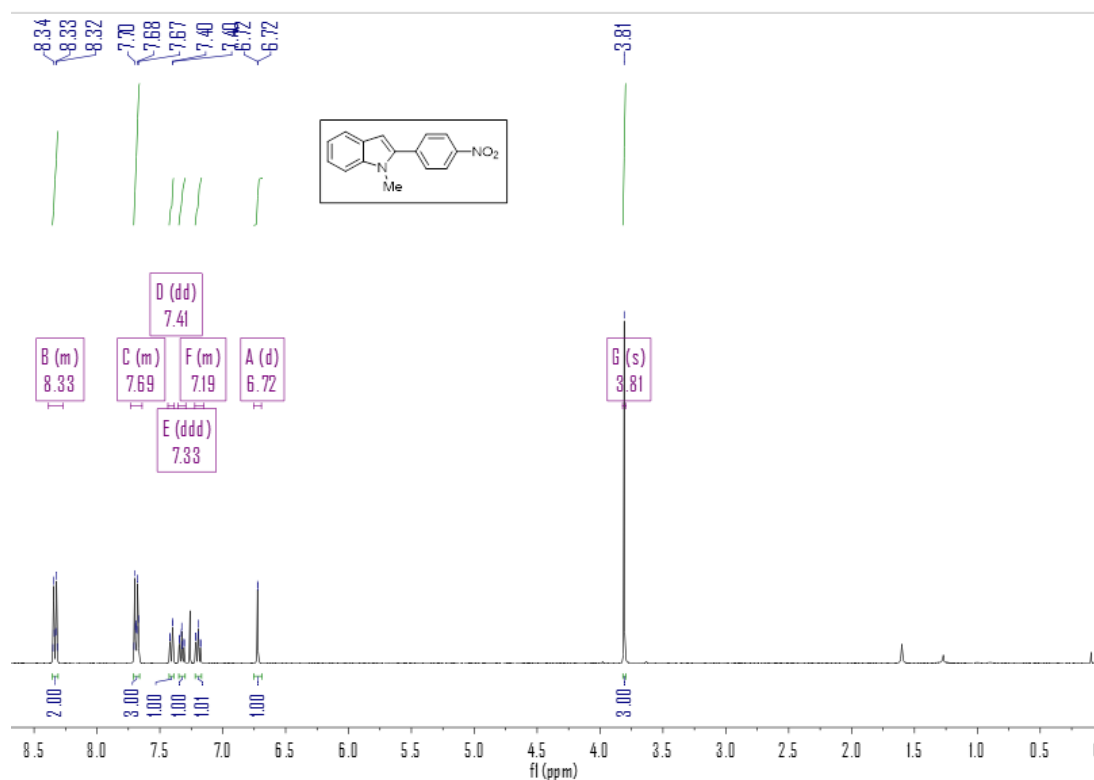


¹³C NMR spectra for **3m**.

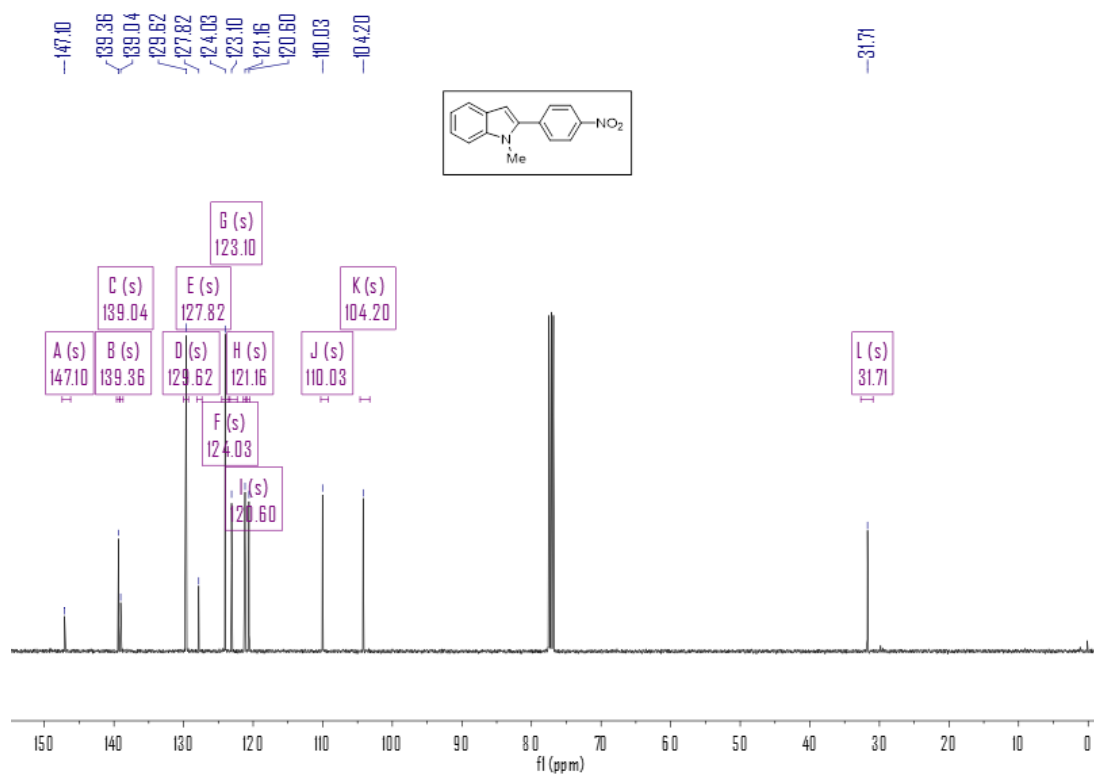


¹⁹F NMR spectra for **3m**.

1-methyl-2-(4-nitrophenyl)-indole (3n)

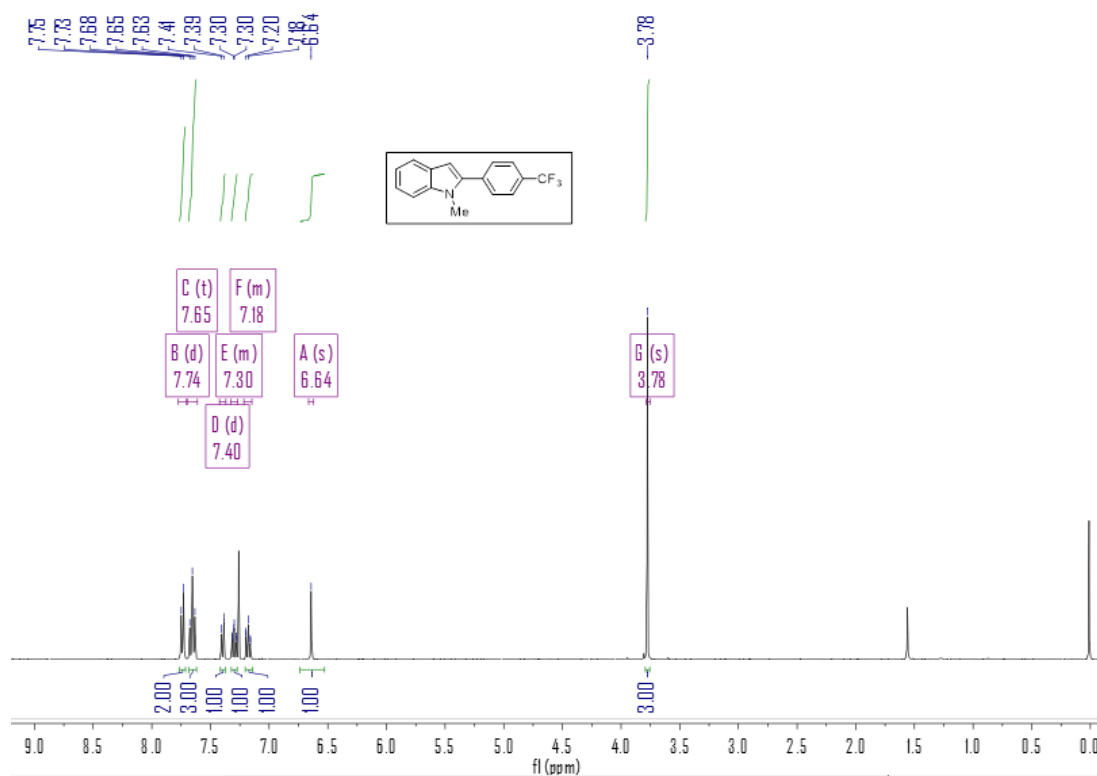


¹H NMR spectra for **3n**.

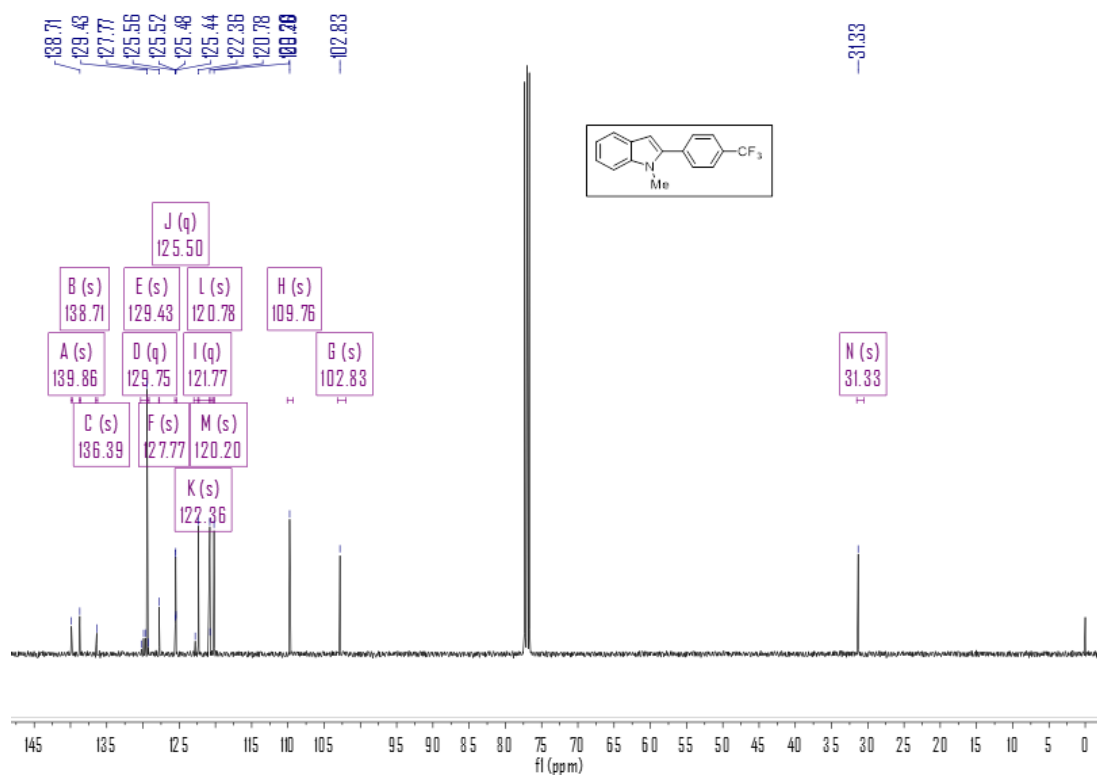


¹³C NMR spectra for **3n**.

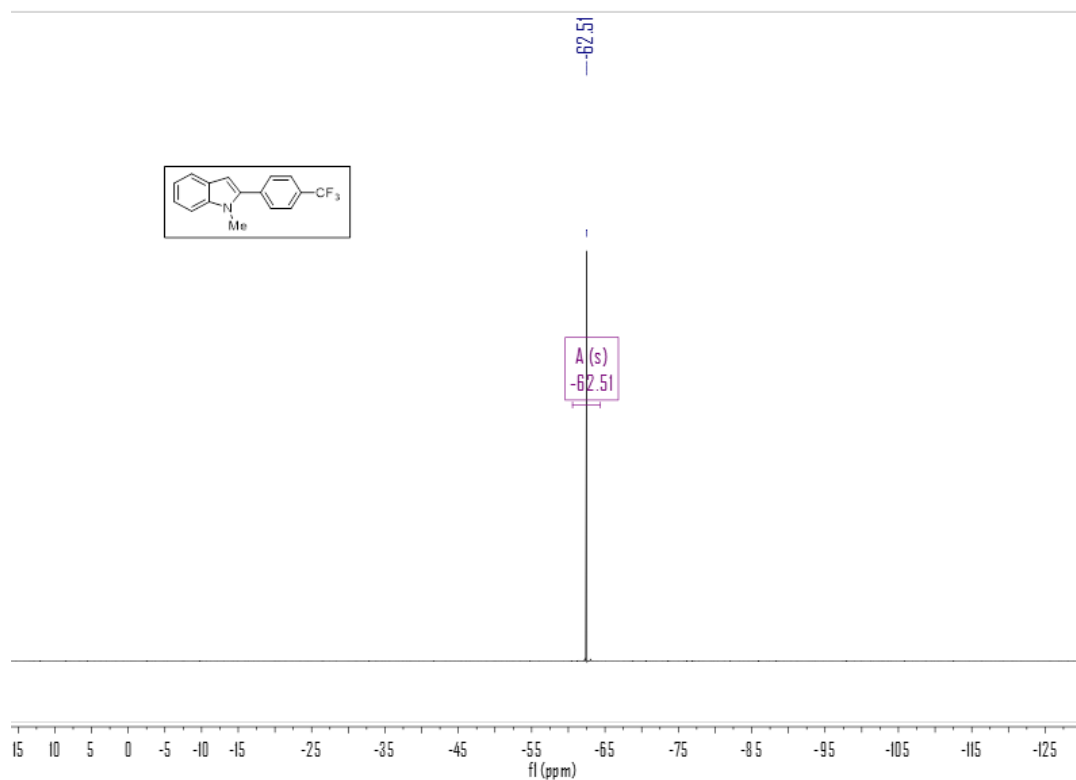
1-methyl-2-(4-(trifluoromethyl)phenyl)-indole (**3o**)



¹H NMR spectra for **3o**.

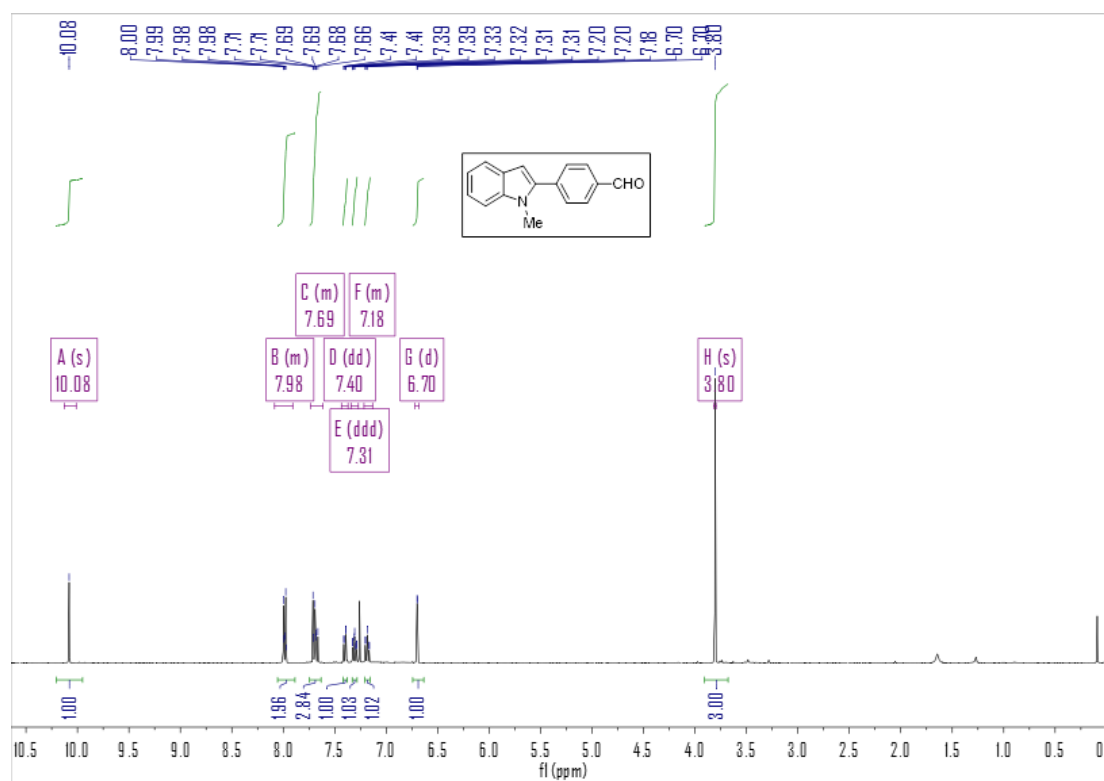


¹³C NMR spectra for **3o**.

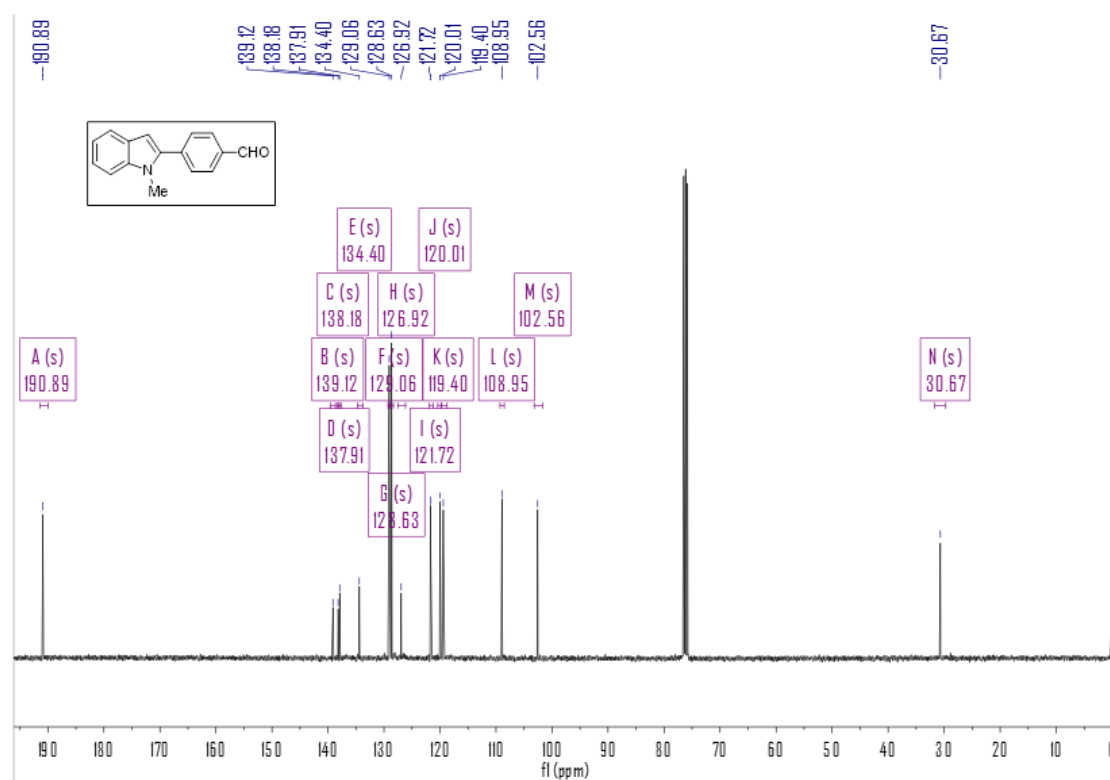


¹⁹F NMR spectra for 3o.

4-(1-methylindol-2-yl)benzaldehyde (3p)

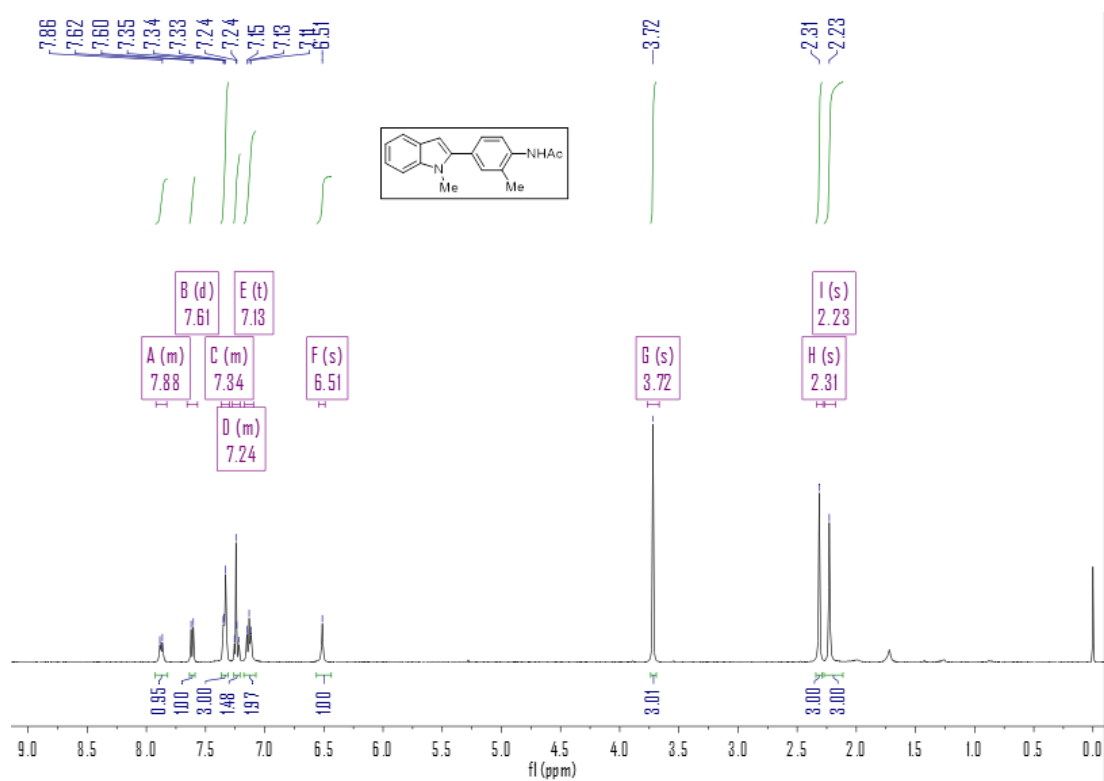


¹H NMR spectra for 3p.

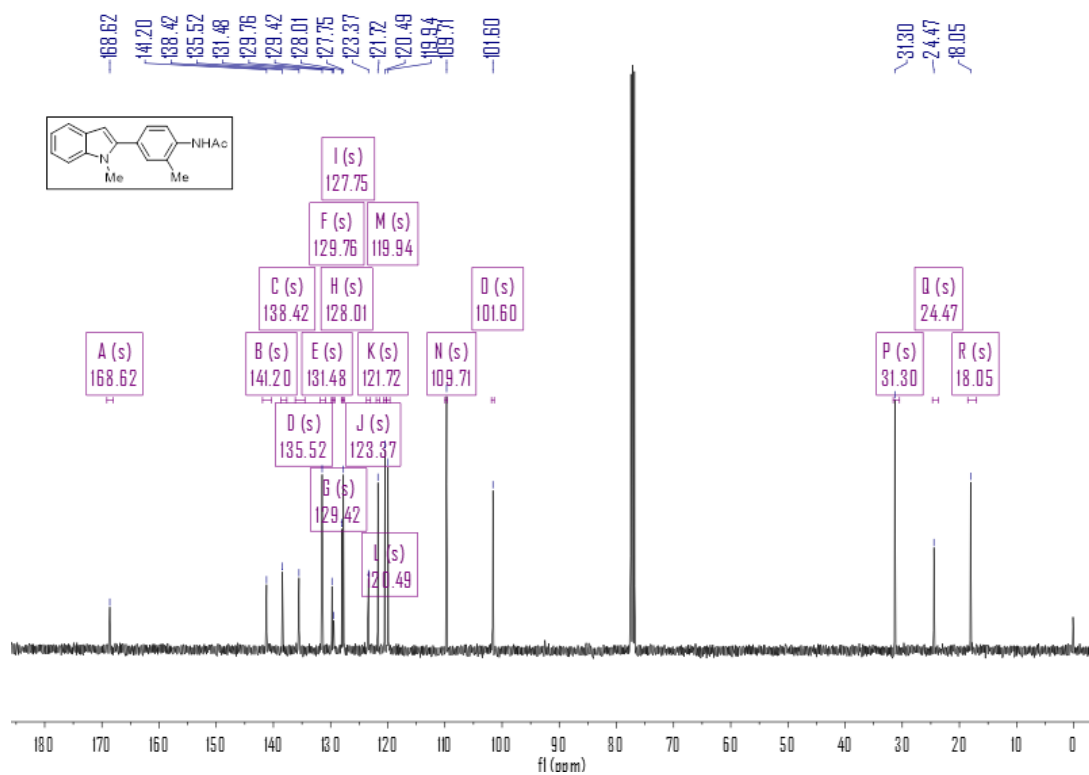


¹³C NMR spectra for **3p**.

N-(2-methyl-4-(1-methylindol-2-yl)phenyl)acetamide (3q)

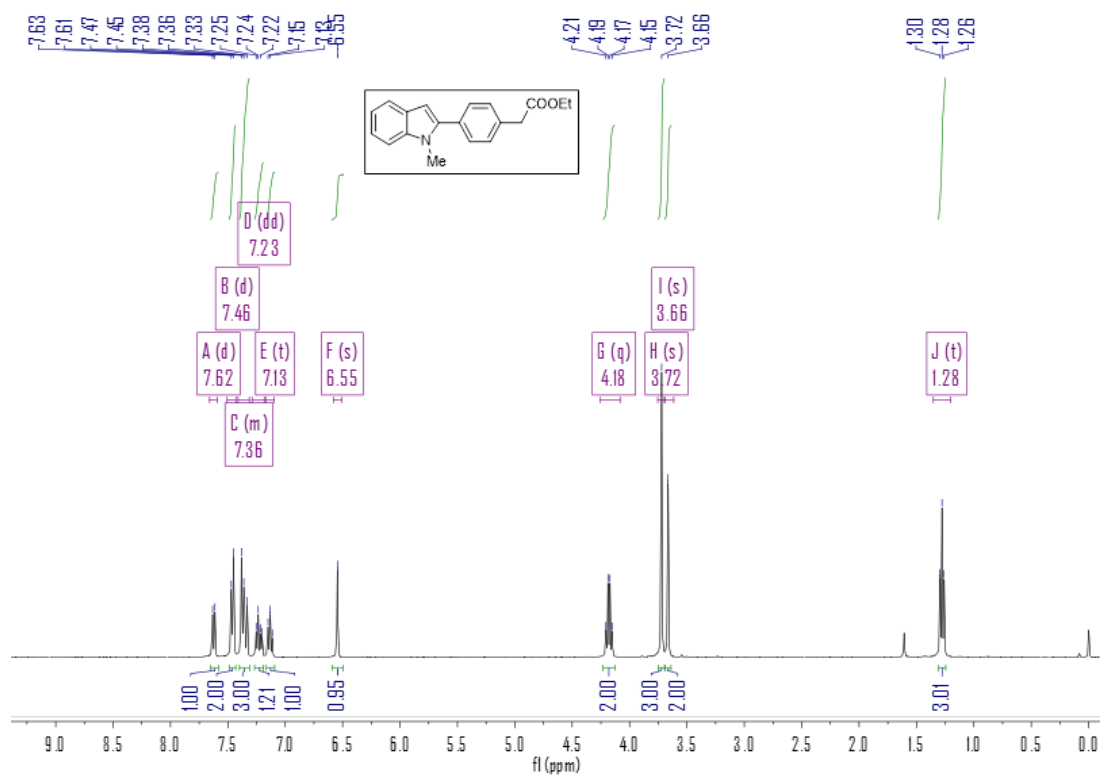


¹H NMR spectra for **3q**.

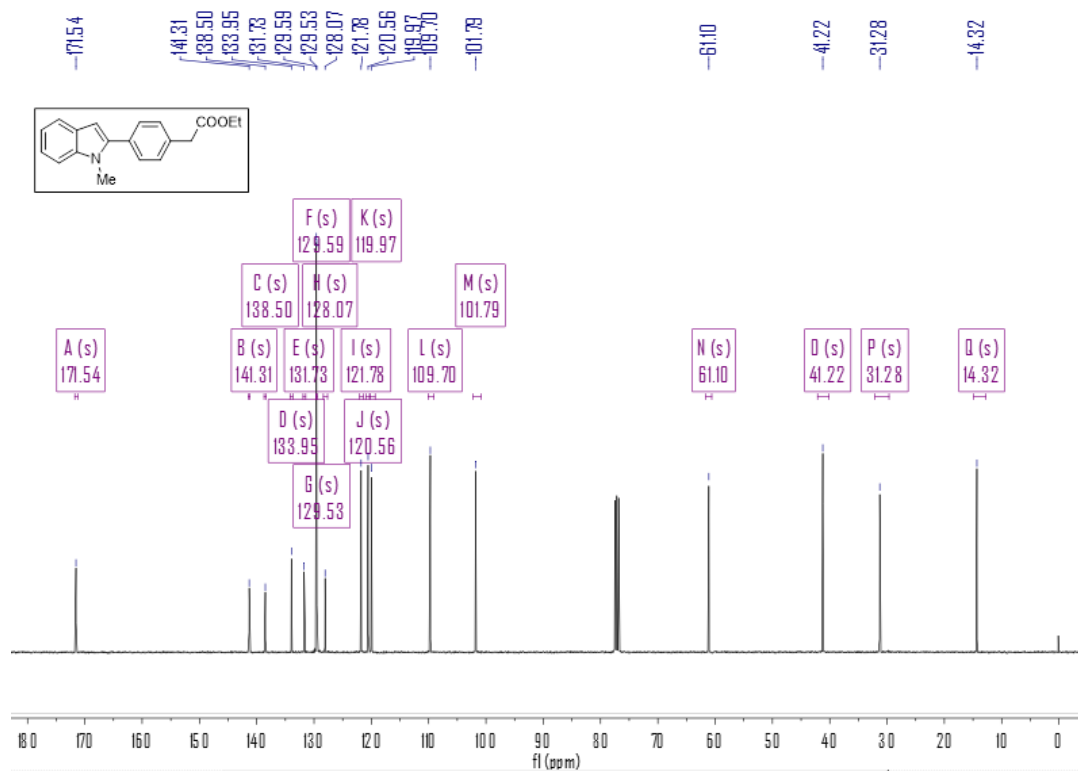


¹³C NMR spectra for **3q**.

ethyl 2-(4-(1-methylindol-2-yl)phenyl)acetate (3r)

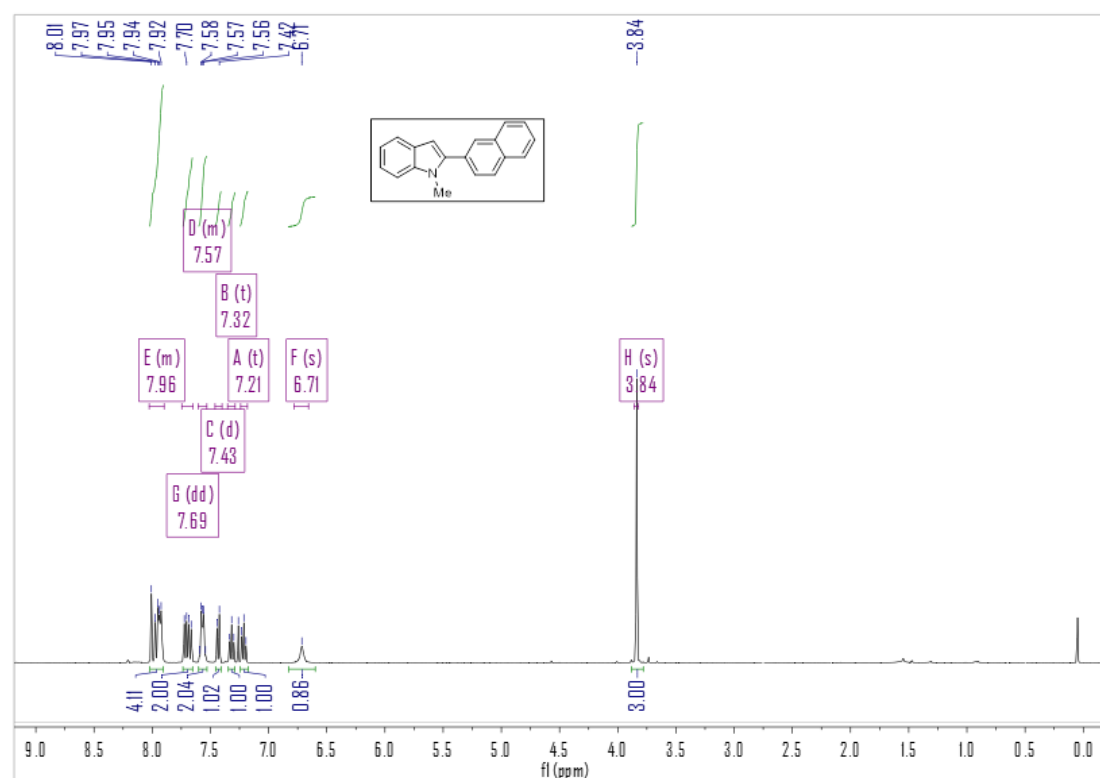


¹H NMR spectra for **3r**.

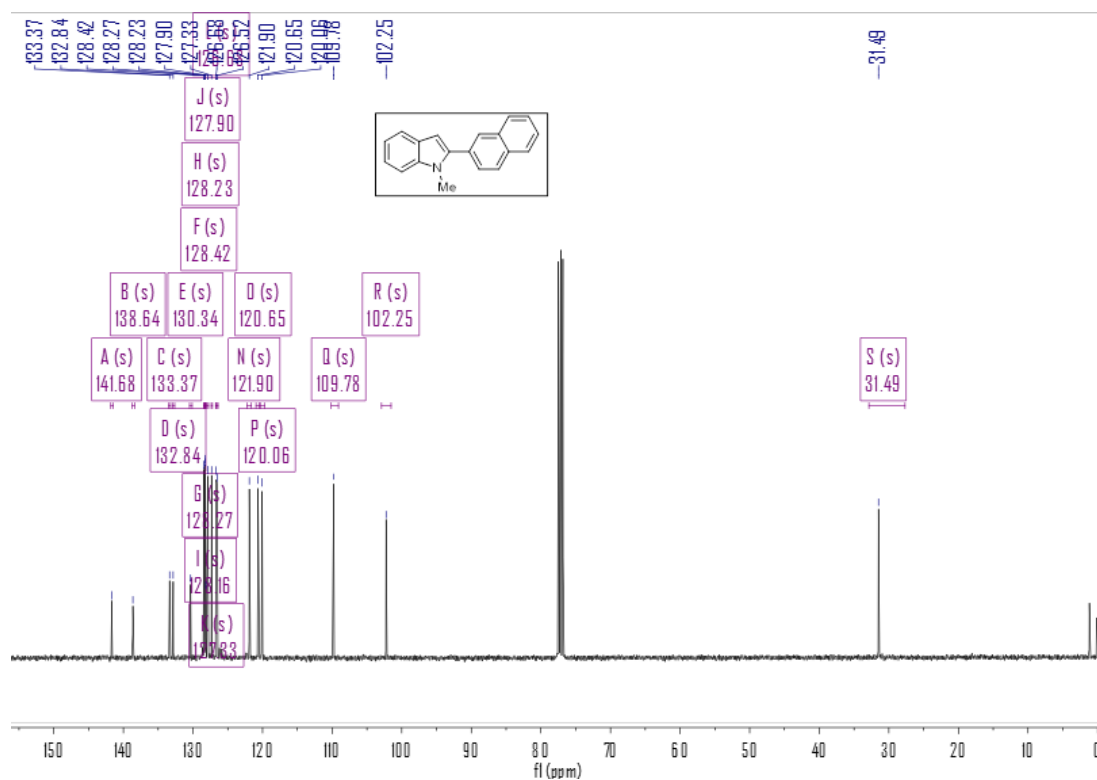


¹³C NMR spectra for 3r.

1-methyl-2-(naphthalen-2-yl)indole (3s)

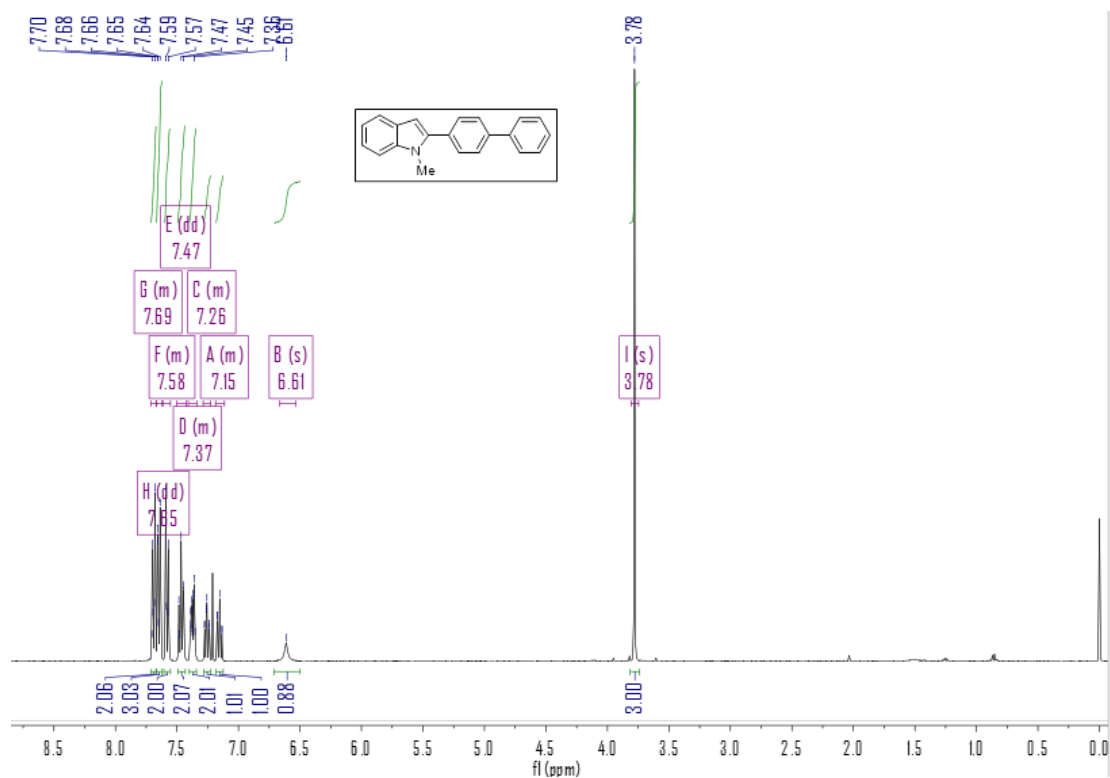


¹H NMR spectra for 3s.

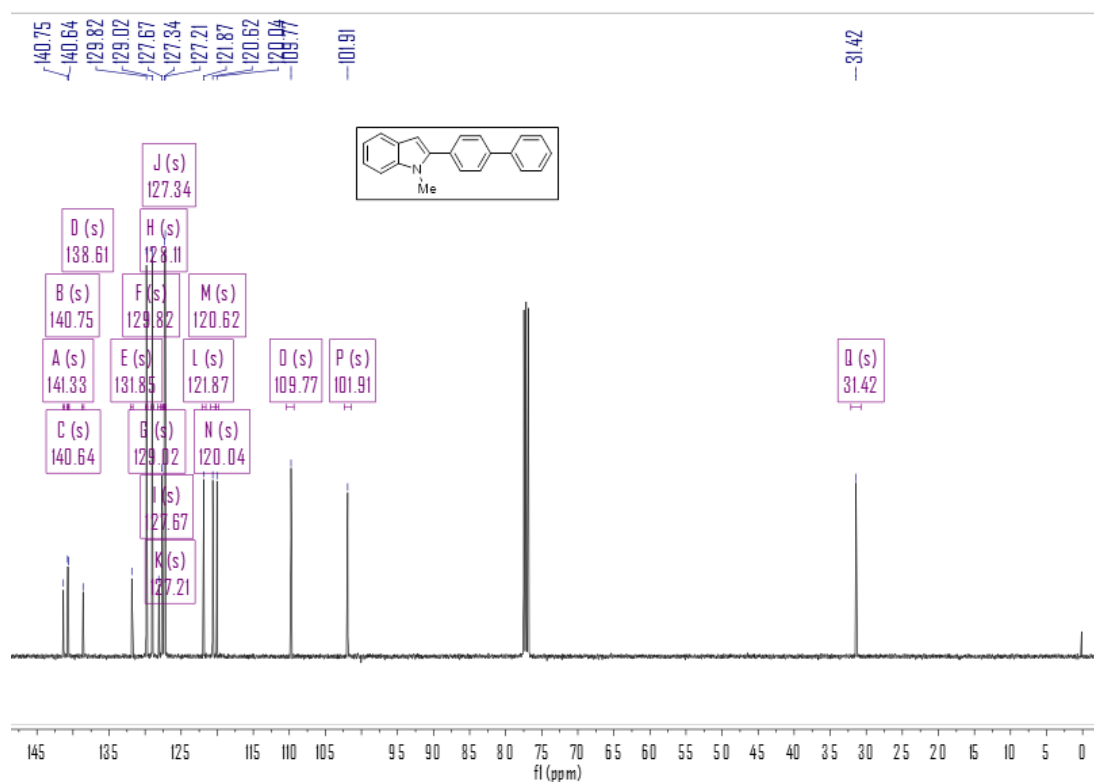


¹³C NMR spectra for **3s**.

2-([1,1'-biphenyl]-4-yl)-1-methylindole (3t**)**

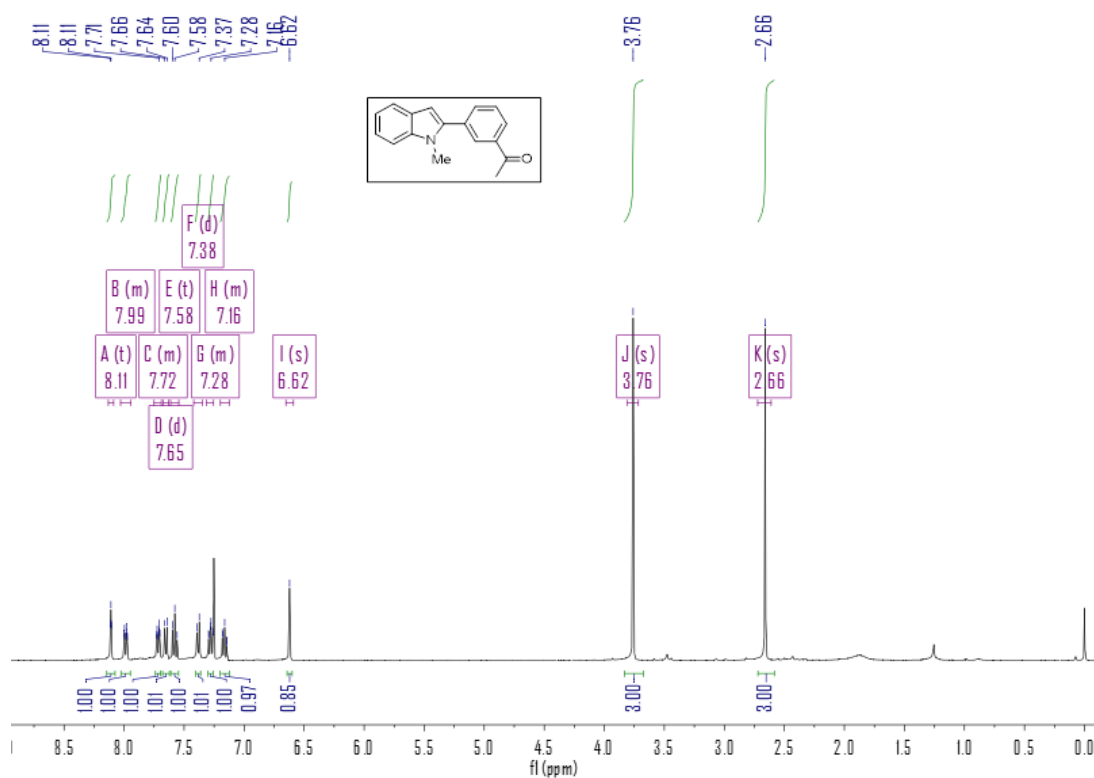


¹H NMR spectra for **3t**.

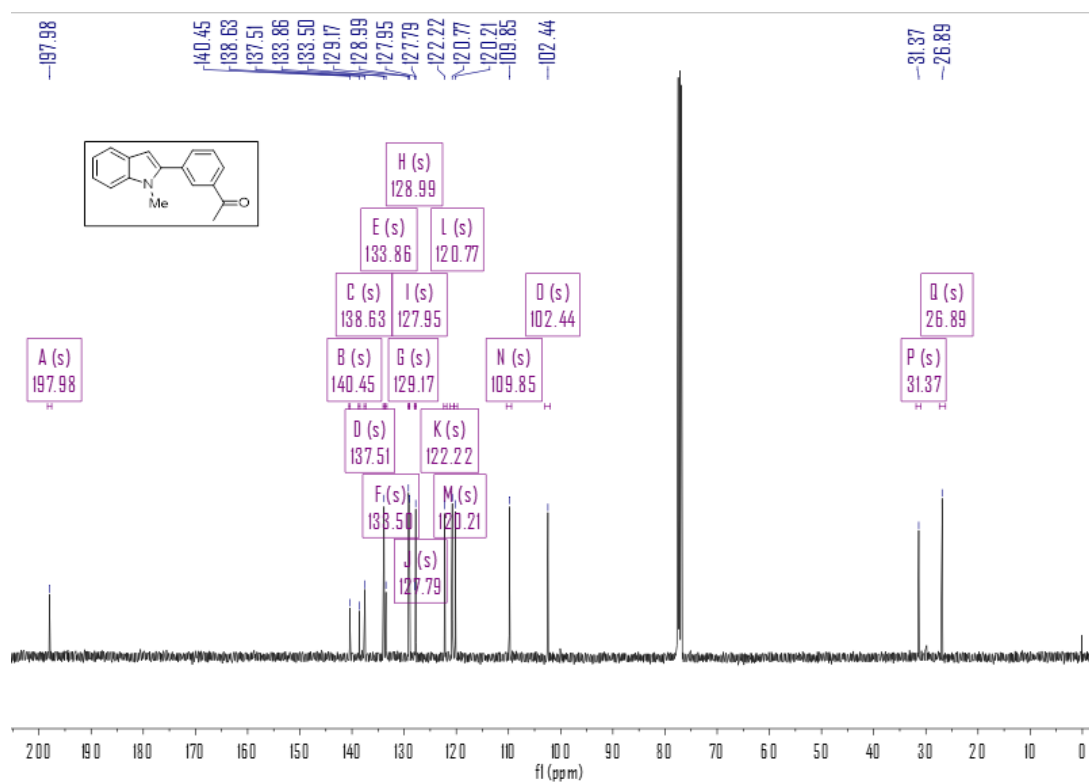


¹³C NMR spectra for **3t**.

1-(3-(1-methylindol-2-yl)phenyl)ethan-1-one (3u)

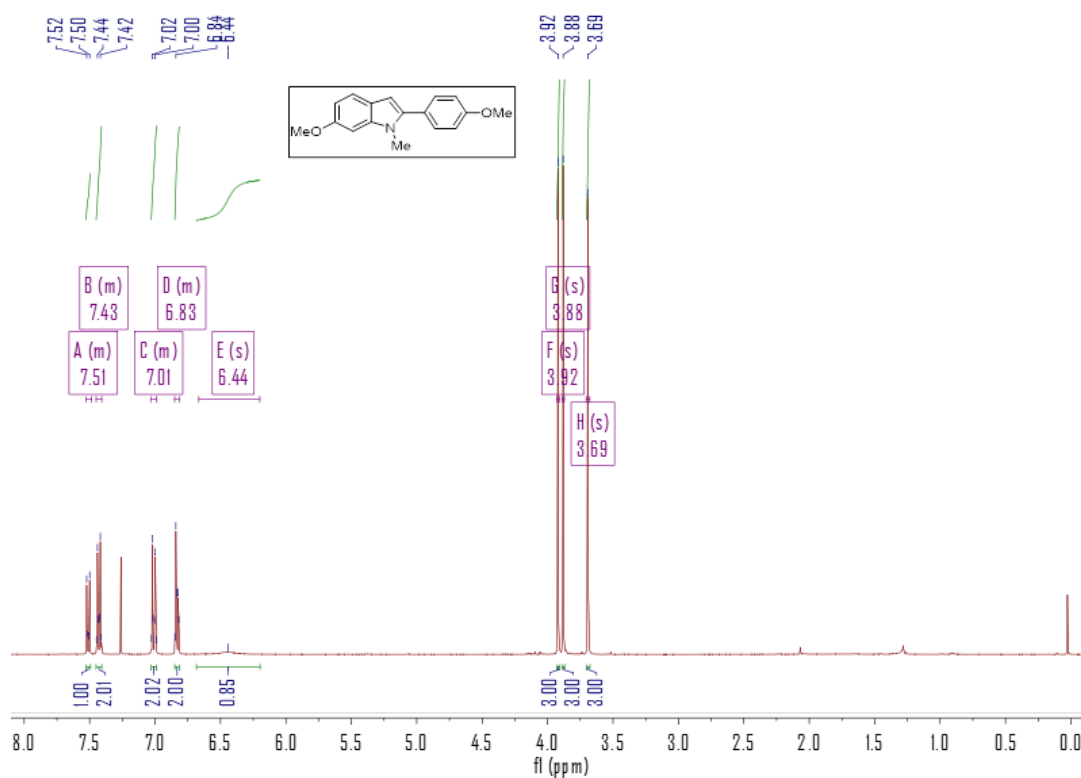


¹H NMR spectra for **3u**.

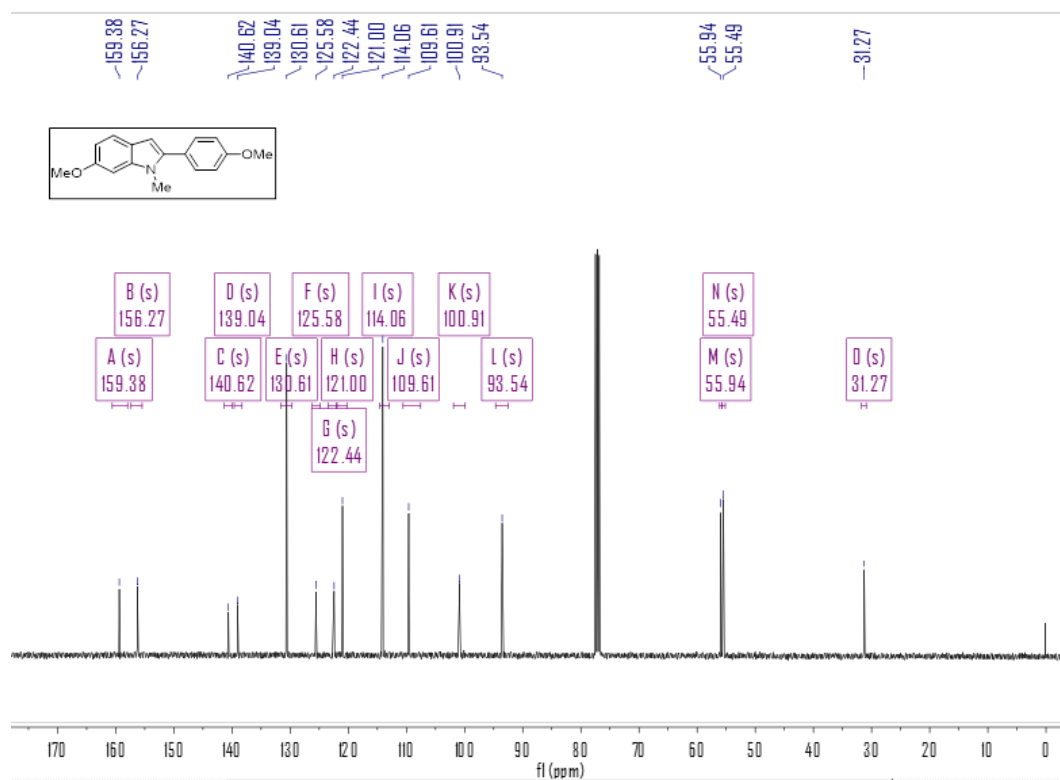


¹³C NMR spectra for **3u**.

6-methoxy-2-(4-methoxyphenyl)-1-methylindole (3v)

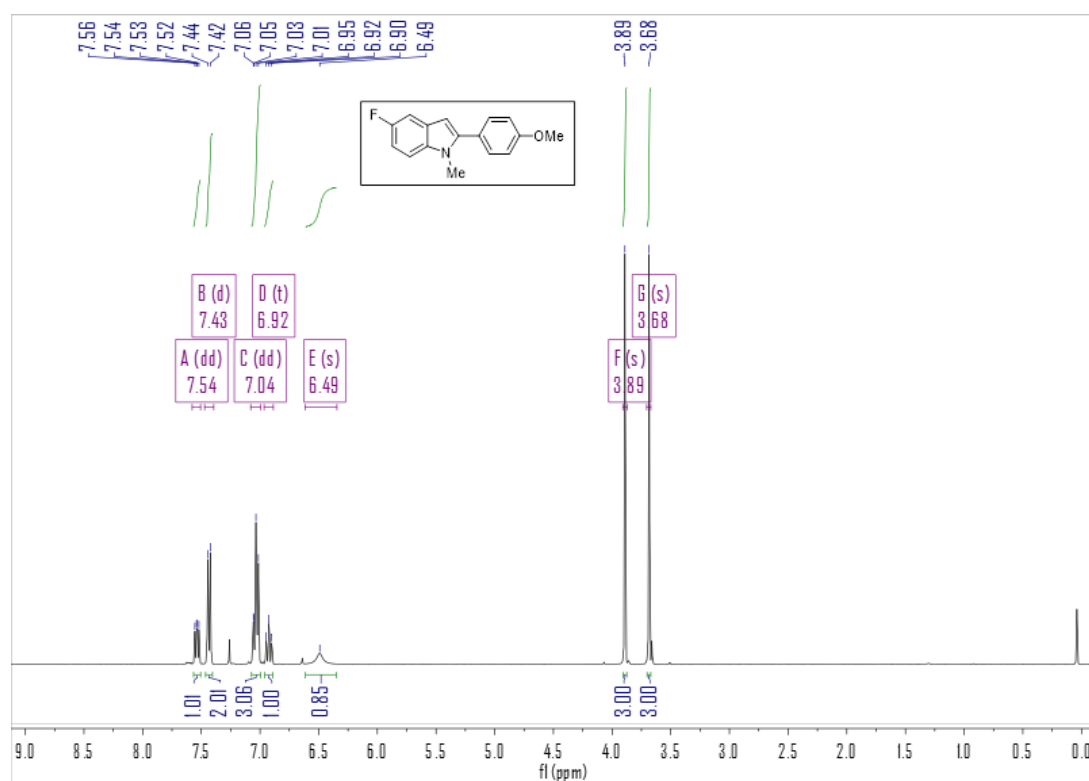


¹H NMR spectra for **3v**.

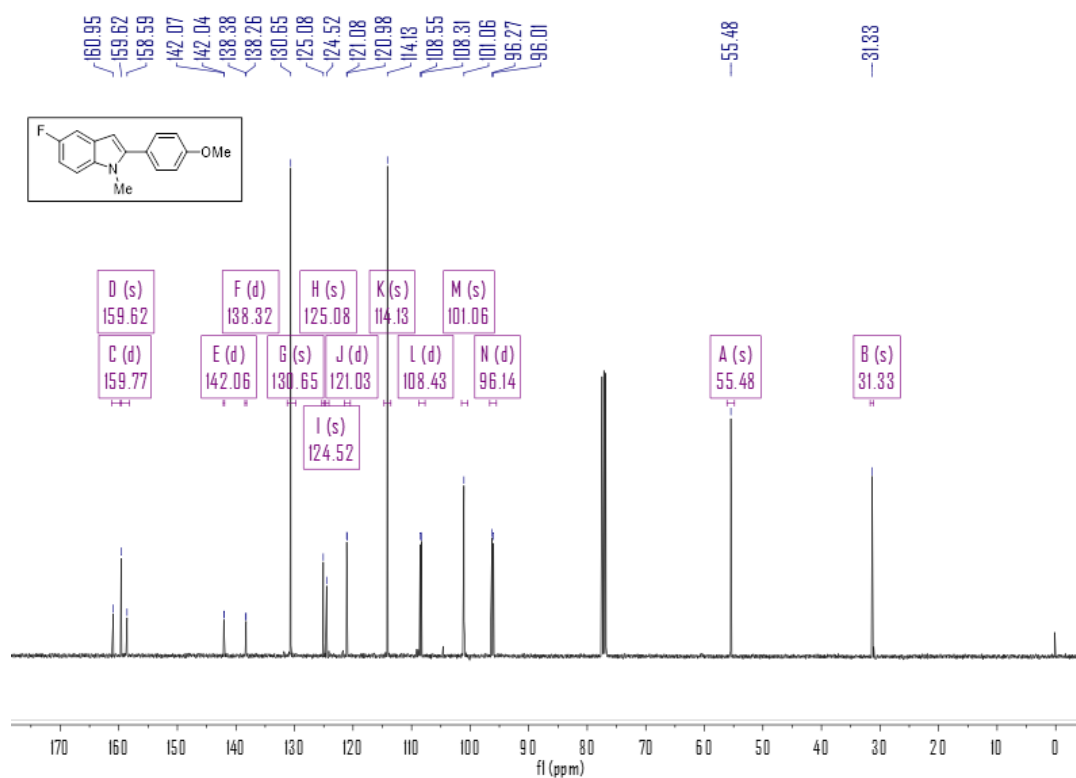


¹³C NMR spectra for **3v**.

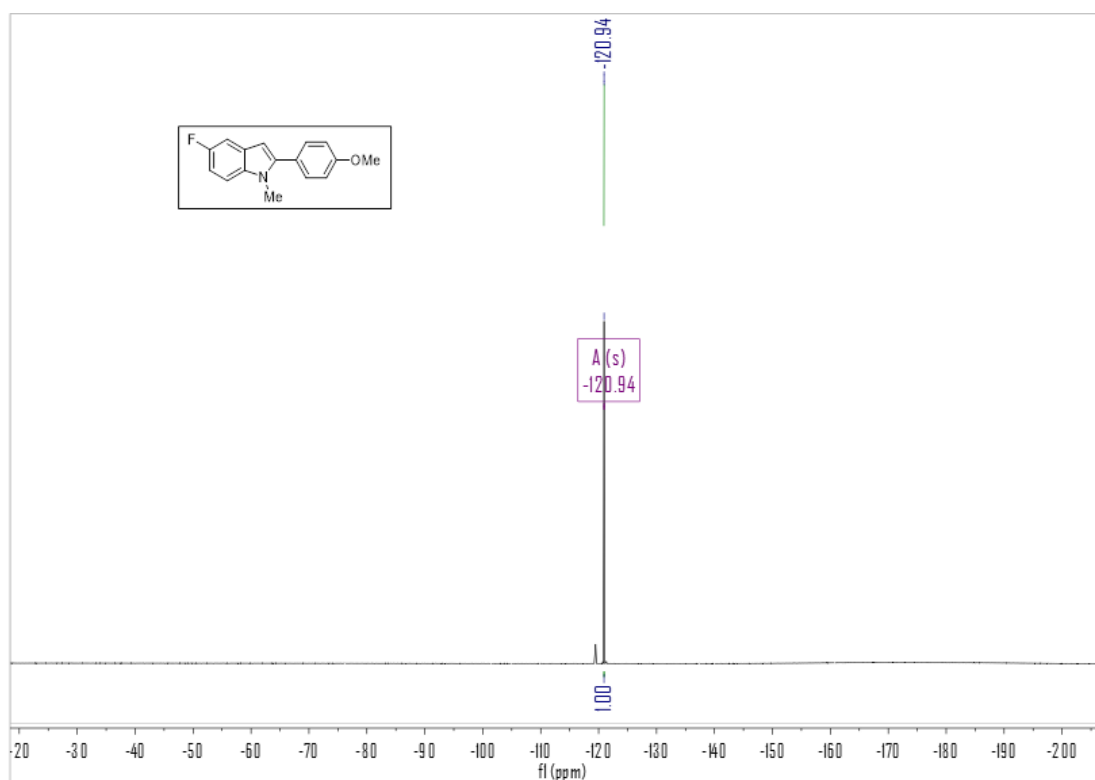
5-fluoro-2-(4-methoxyphenyl)-1-methylindole (**3w**)



¹H NMR spectra for **3w**.

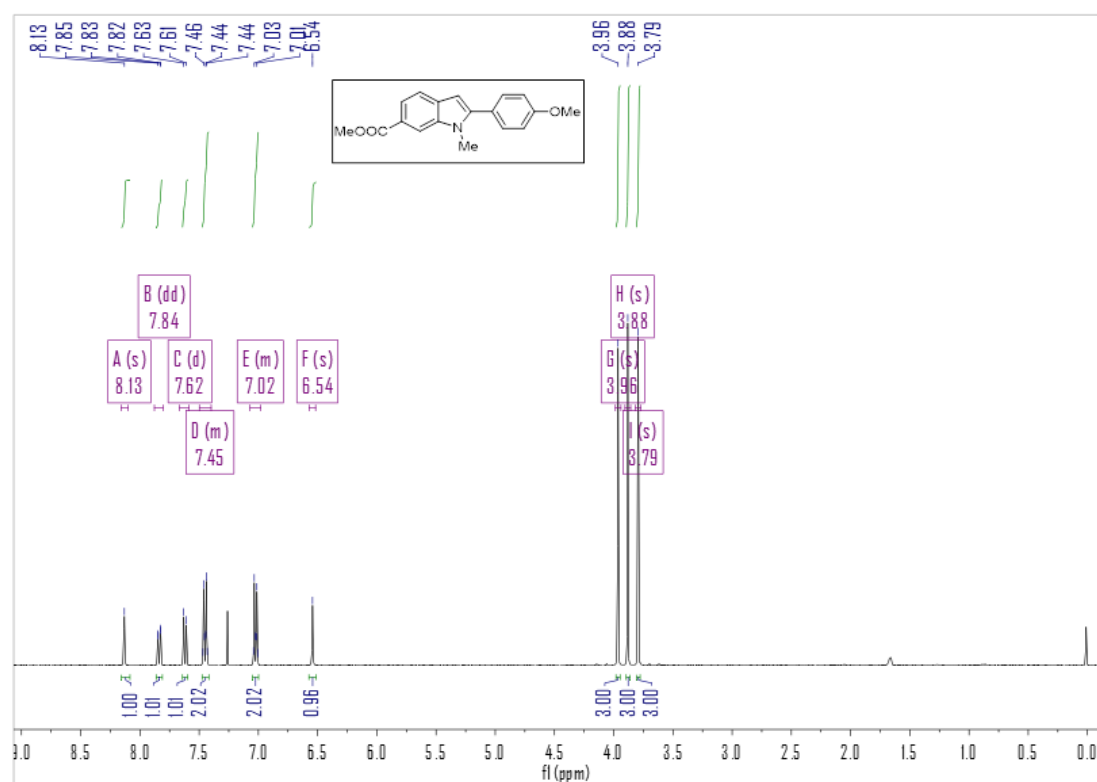


¹³C NMR spectra for **3w**.

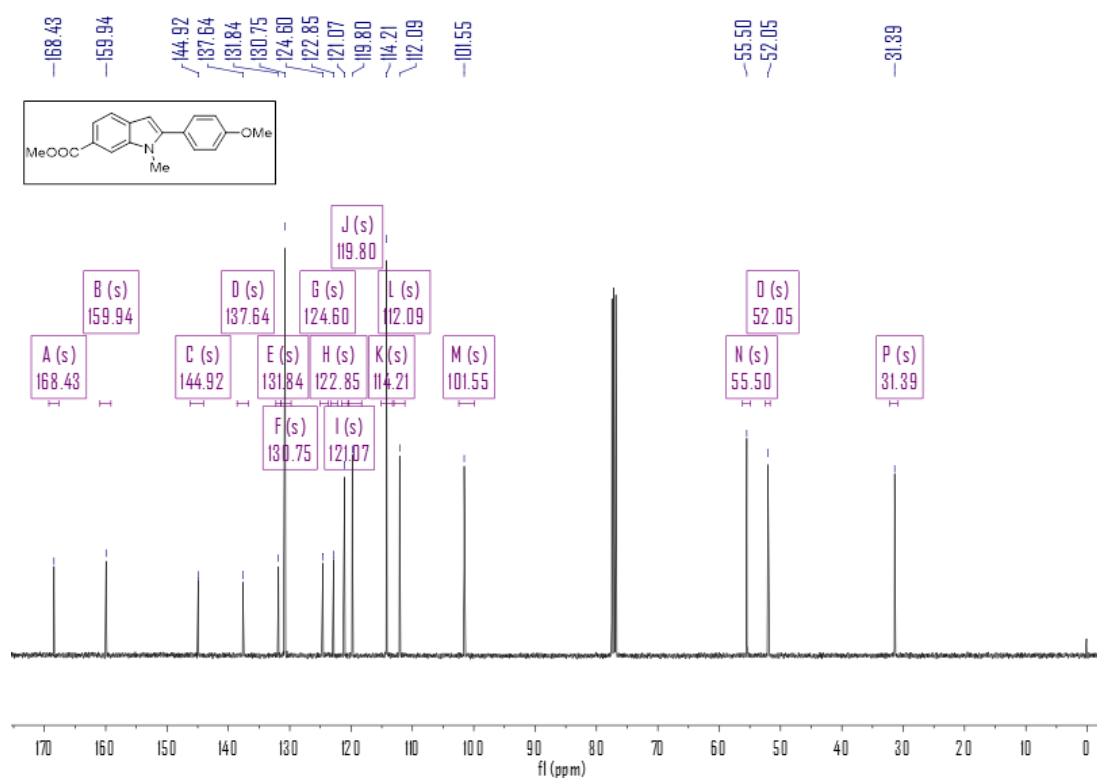


¹⁹F NMR spectra for **3w**.

methyl 2-(4-methoxyphenyl)-1-methylindole-6-carboxylate (3x)

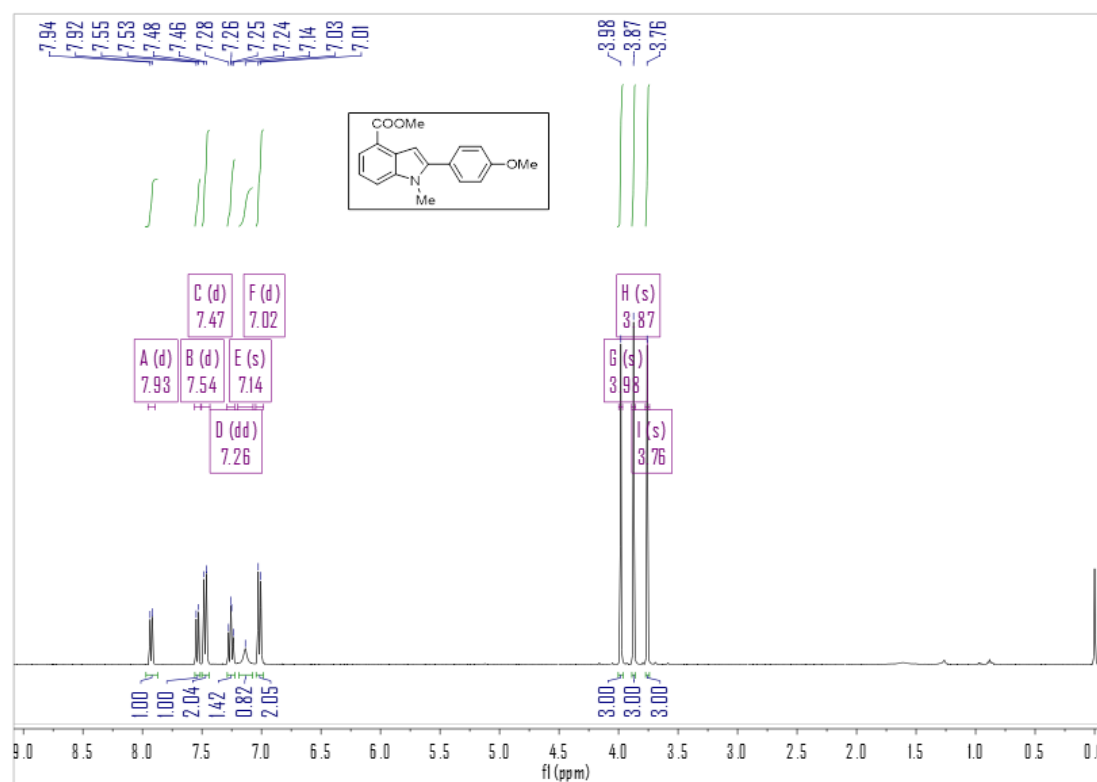


¹H NMR spectra for **3x**.

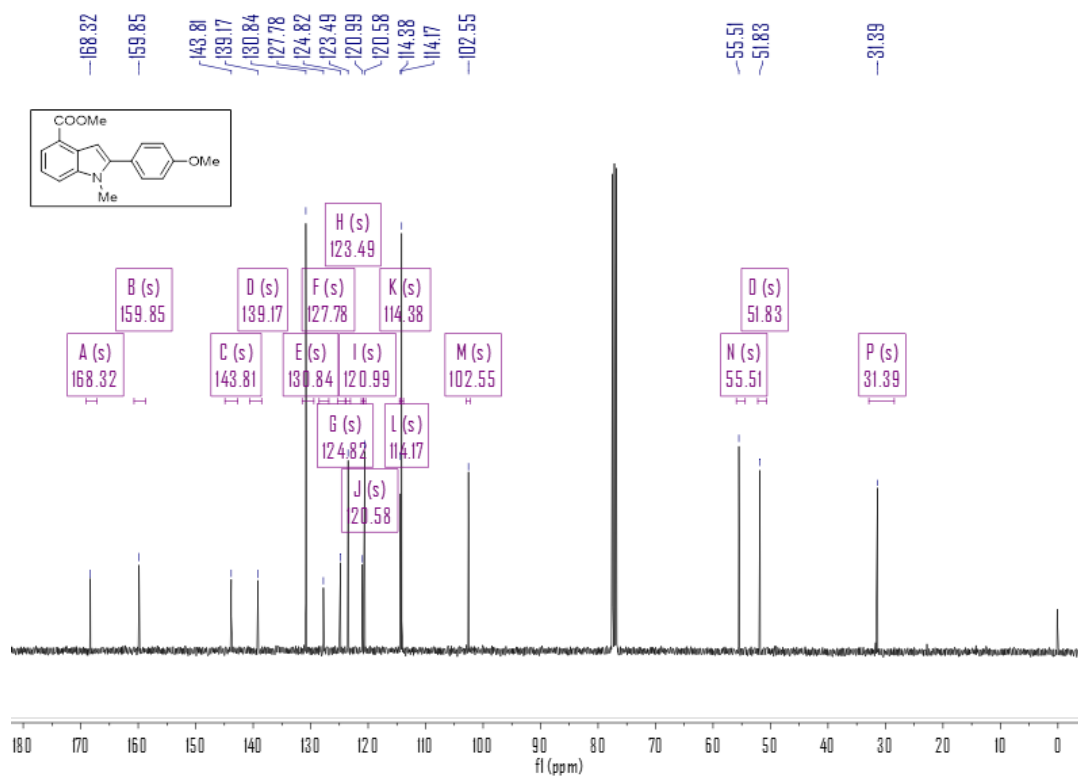


¹³C NMR spectra for **3x**.

methyl 2-(4-methoxyphenyl)-1-methylindole-4-carboxylate (3y)

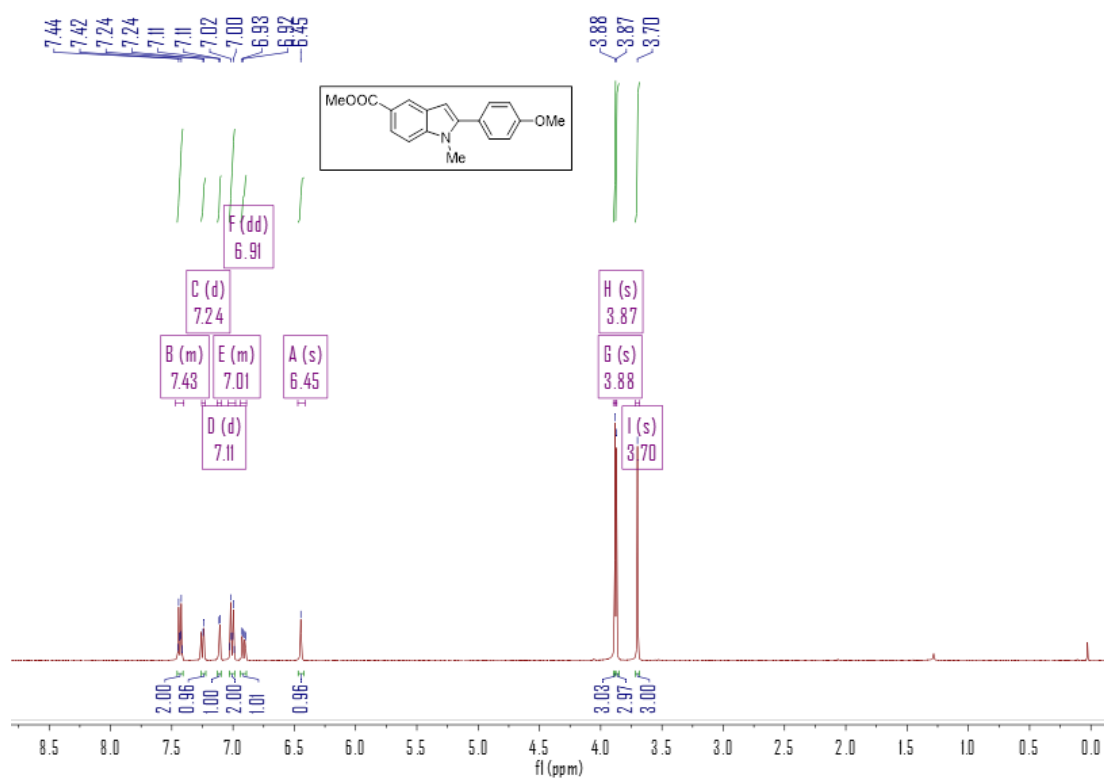


¹H NMR spectra for 3y.

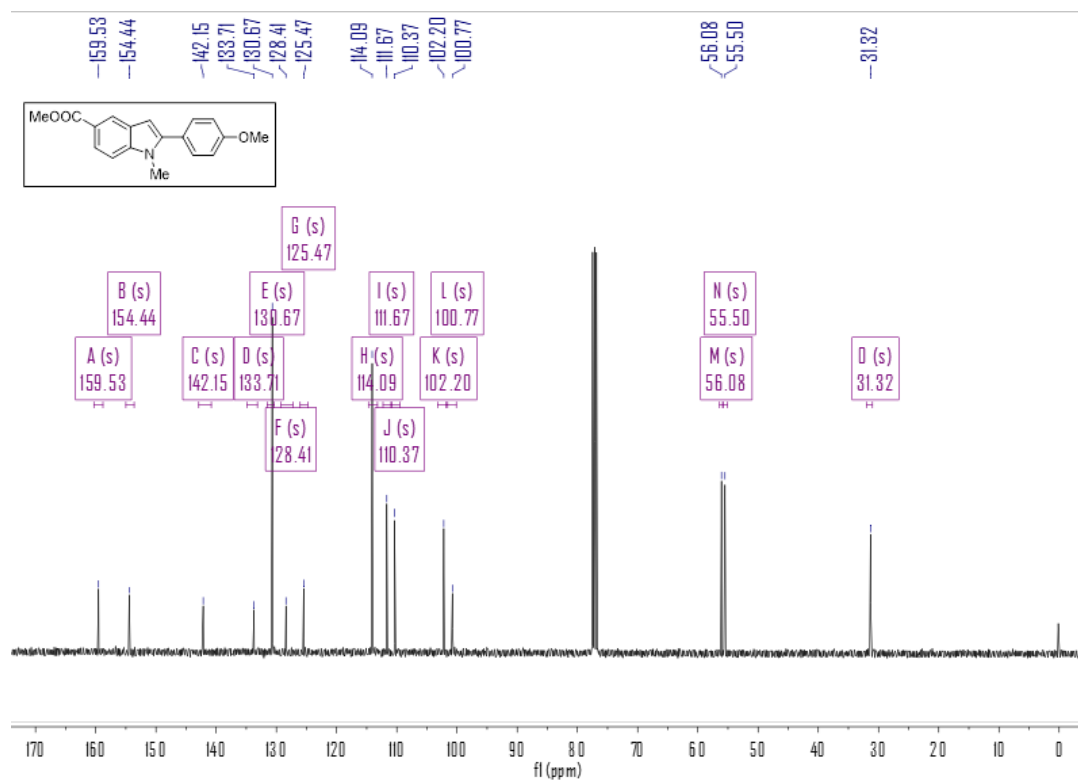


¹³C NMR spectra for 3y.

methyl 2-(4-methoxyphenyl)-1-methylindole-5-carboxylate (3z)

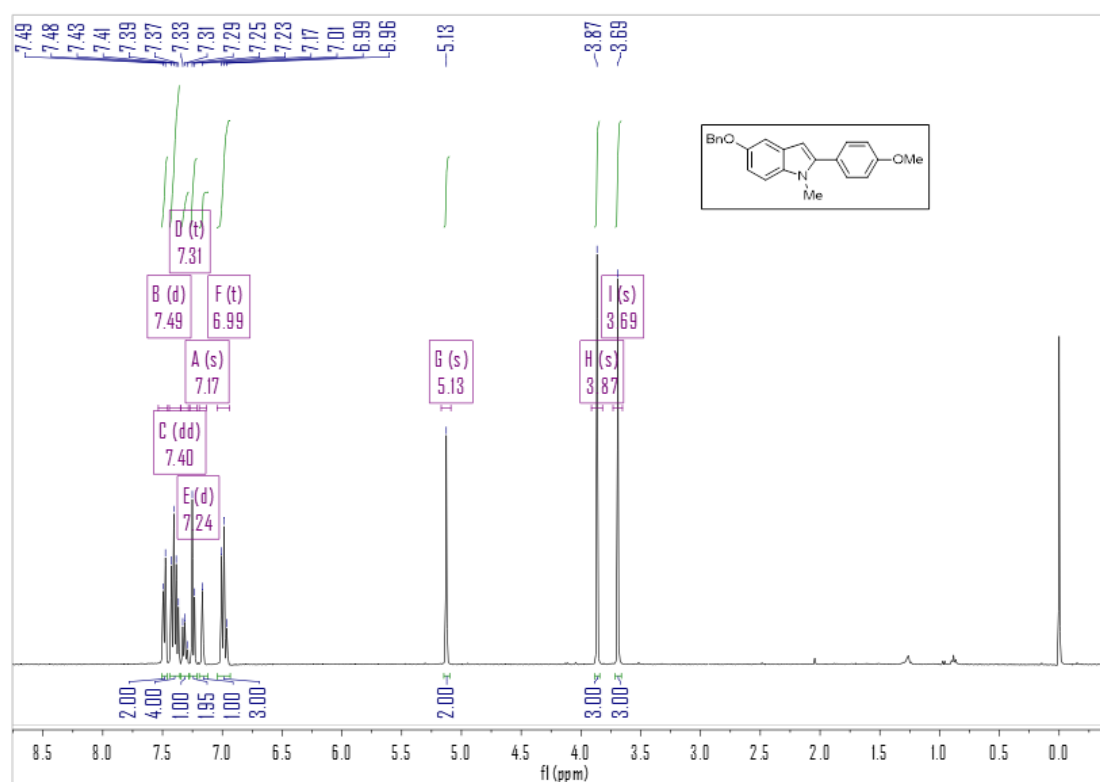


¹H NMR spectra for **3z**.

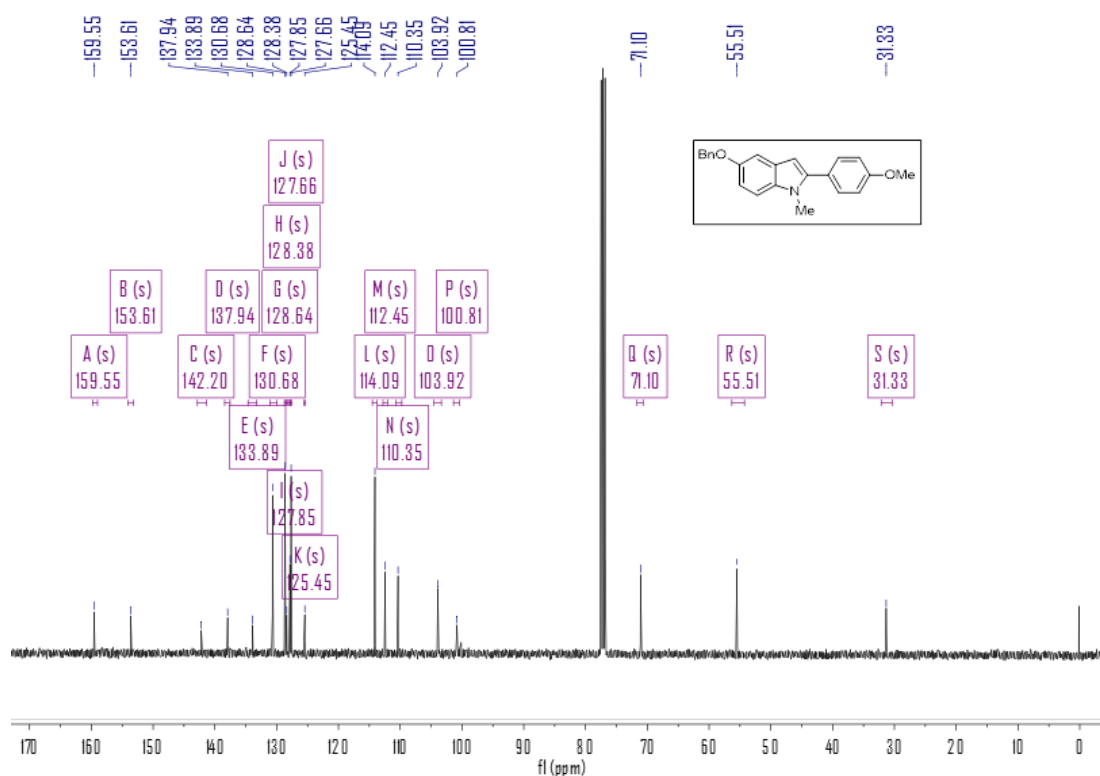


¹³C NMR spectra for **3z**.

5-(benzyloxy)-2-(4-methoxyphenyl)-1-methylindole (3aa)

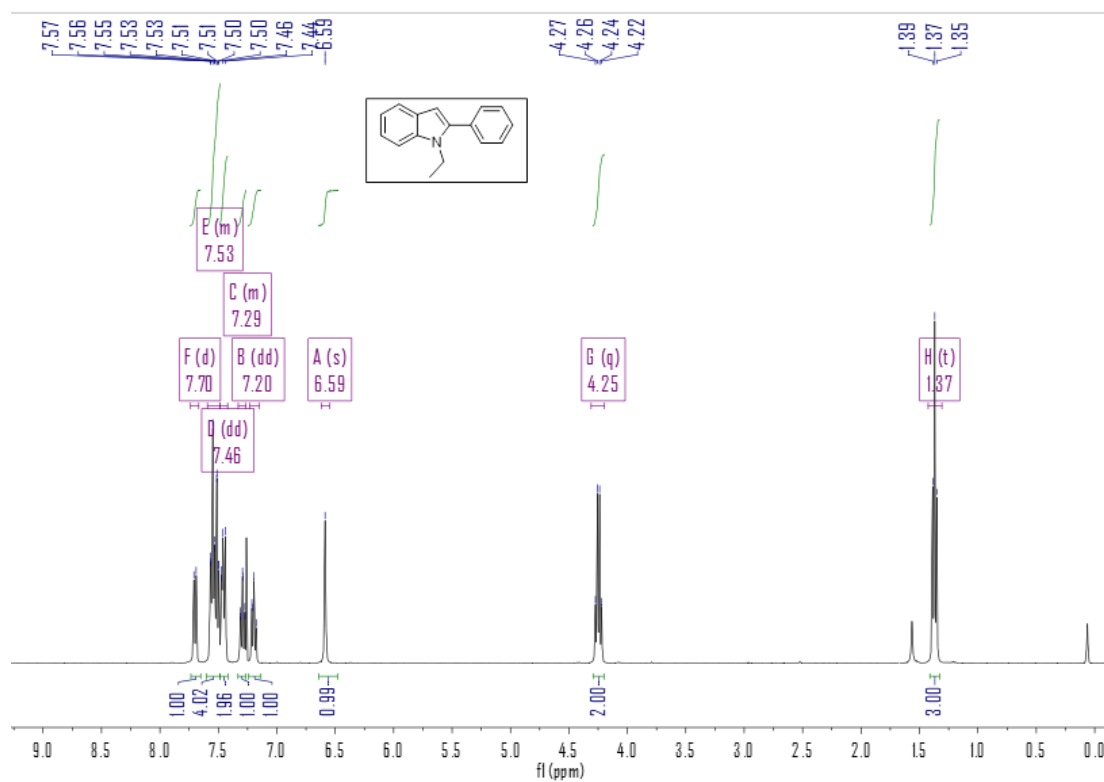


^1H NMR spectra for 3aa.

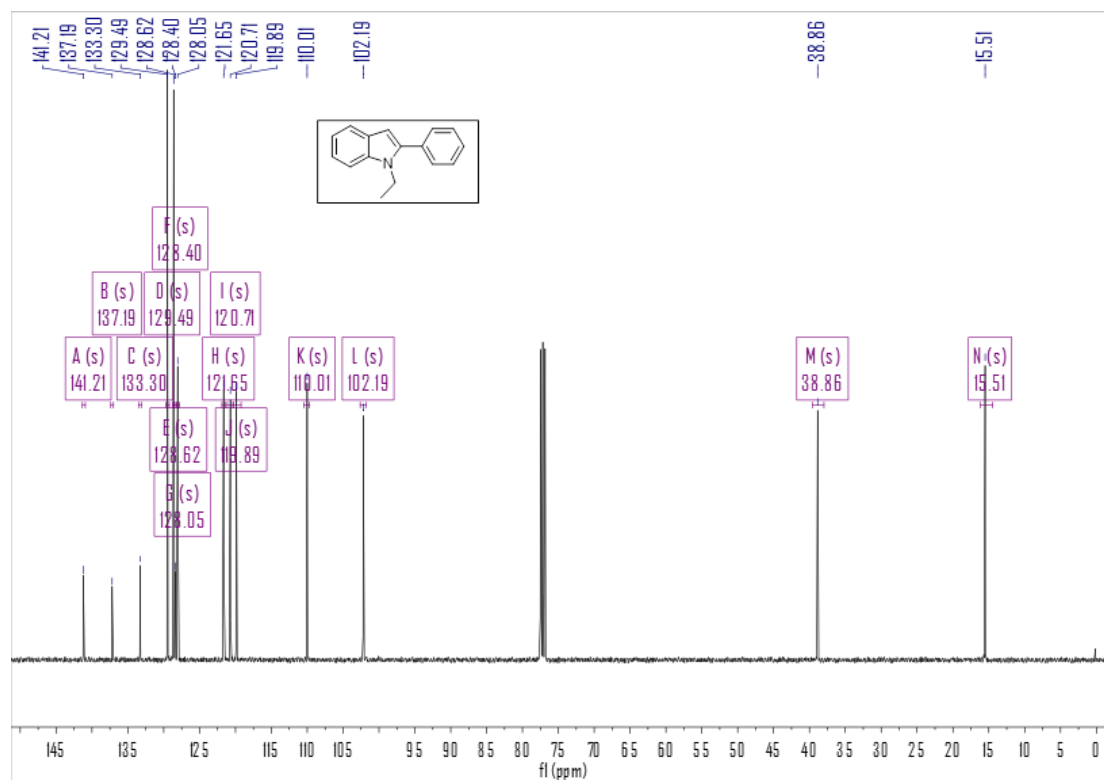


^{13}C NMR spectra for 3aa.

1-ethyl-2-phenylindole (3ab)

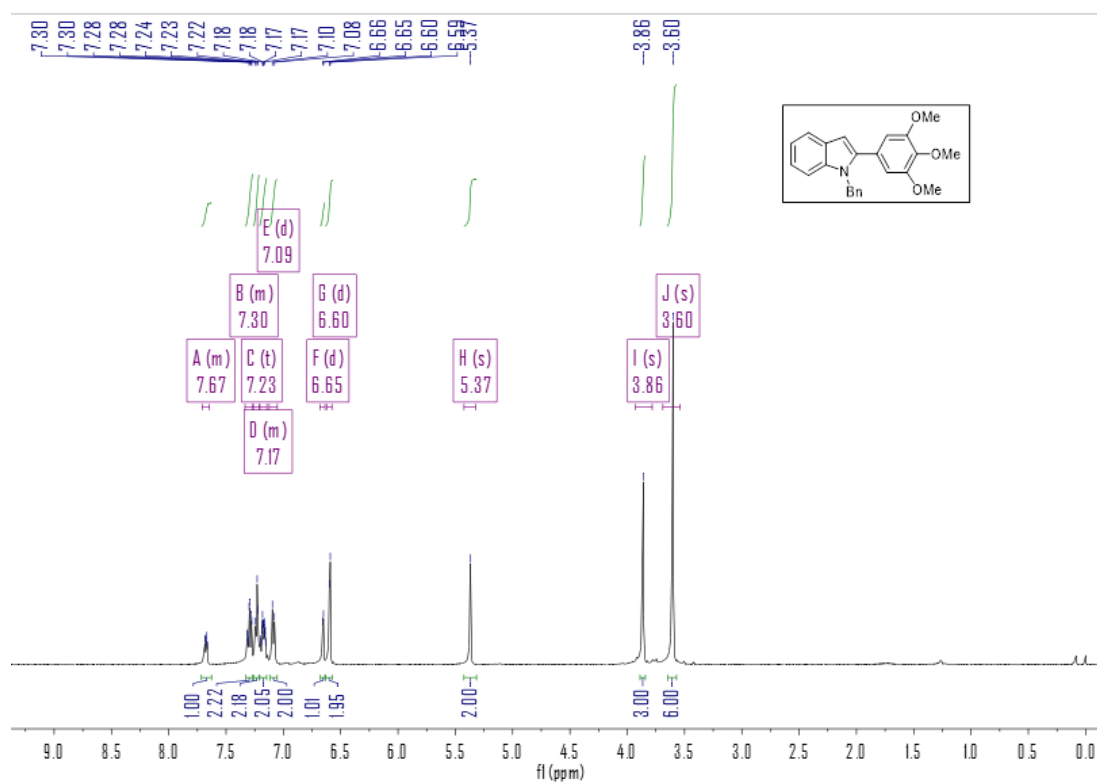


¹H NMR spectra for **3ab**.

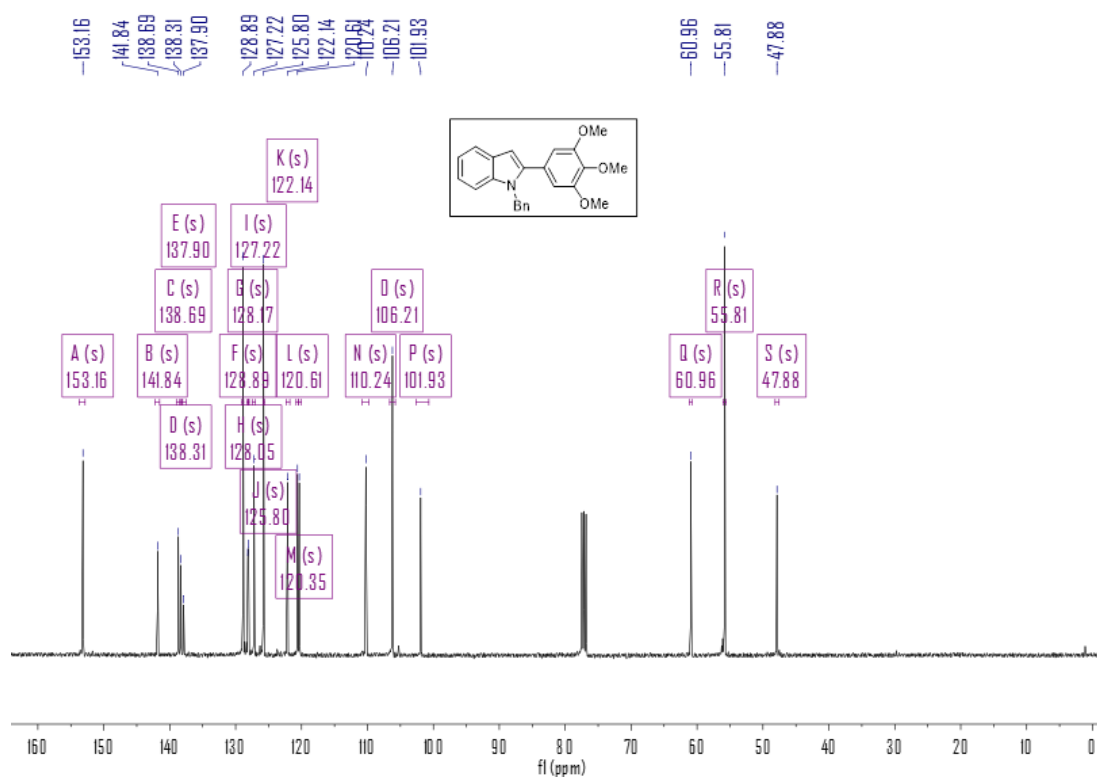


¹³C NMR spectra for **3ab**.

1-benzyl-2-(3,4,5-trimethoxyphenyl)-indole (3ac)



¹H NMR spectra for 3ac.



¹³C NMR spectra for 3ac.