Electronic Supplementary Material (ESI) for RSC Advances.

Support Information

Palladium Schiff-Base Complex Modified Cu(BDC-NH_2) Metal Organic Framework Catalysts for used application in C-N Coupling reaction

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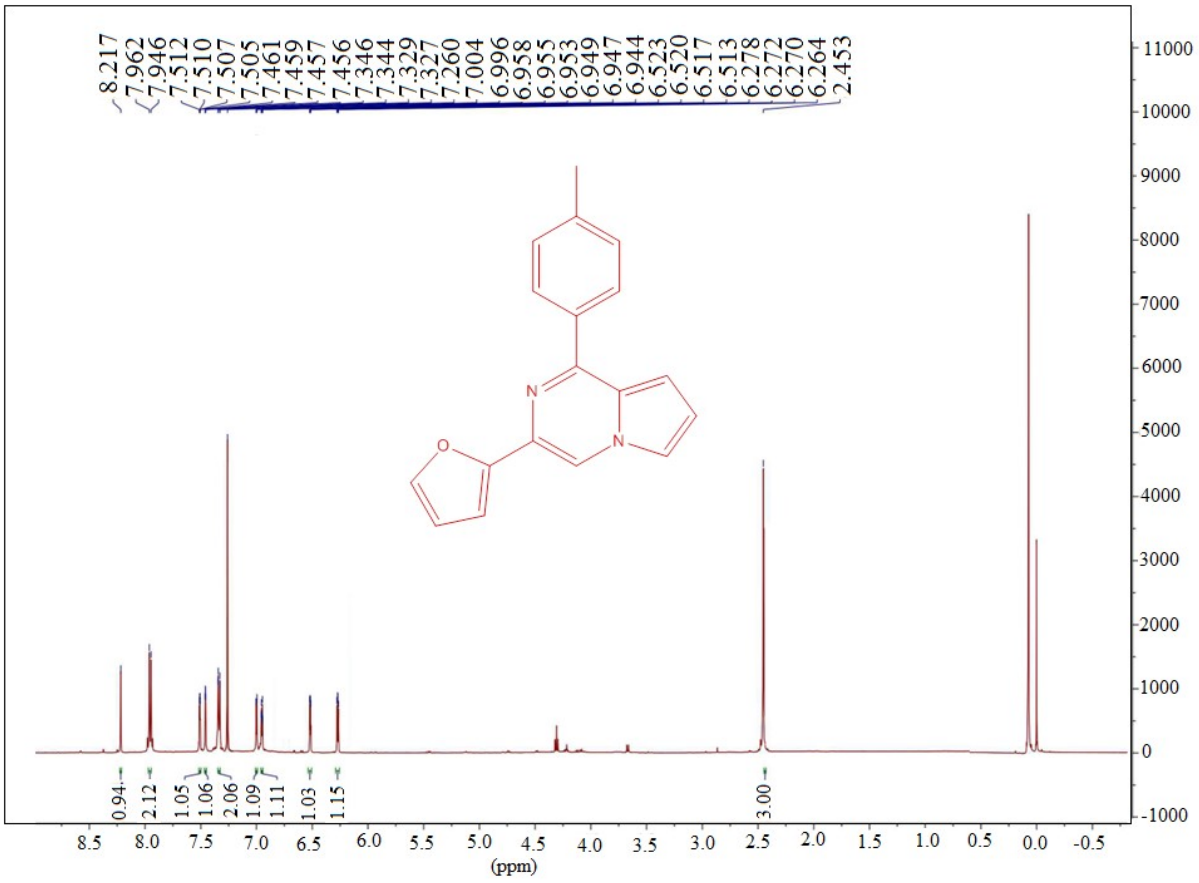
^{1}H NMR Spectrum 3-(furan-2-yl)-1-(p-tolyl)pyrrolo[1,2-a]pyrazine(3a)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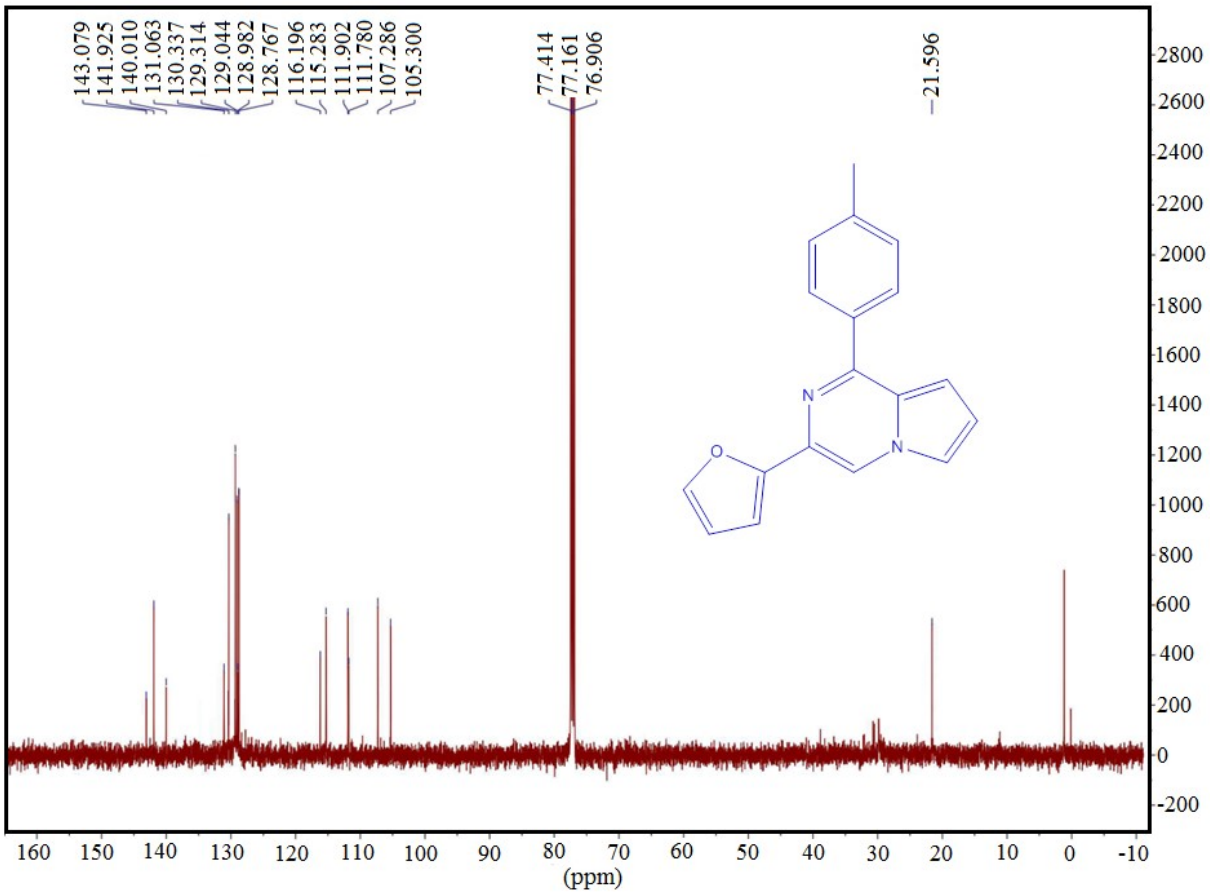
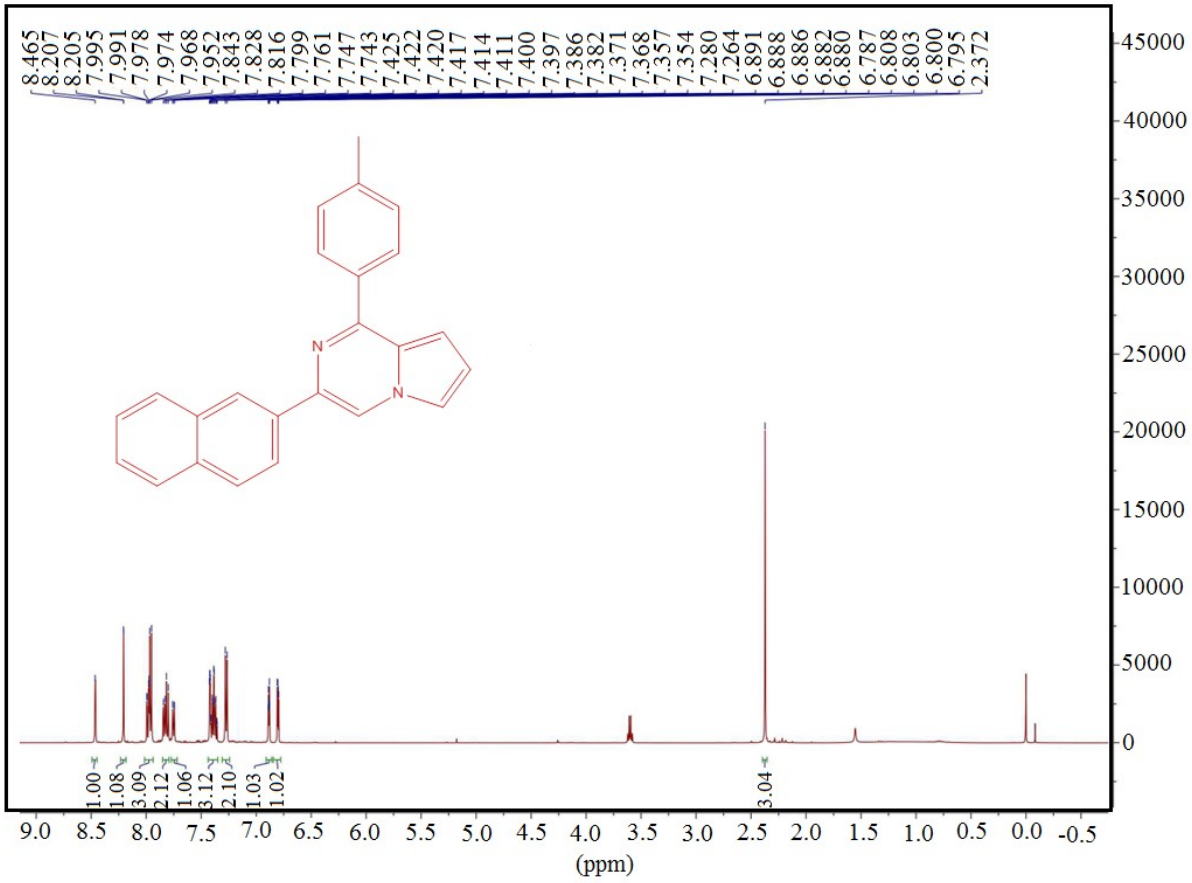
7.344
7.329
7.327
7.260
7.004
6.996
6.958
6.955
6.953
6.949
6.947
6.944
6.523
6.520
6.517
6.513
6.278
6.272
6.270
6.264
2.453
N
O
N
0.94
2.12
1.05
1.06
2.06
1.09
1.11
1.03
1.15
3.00
(ppm)

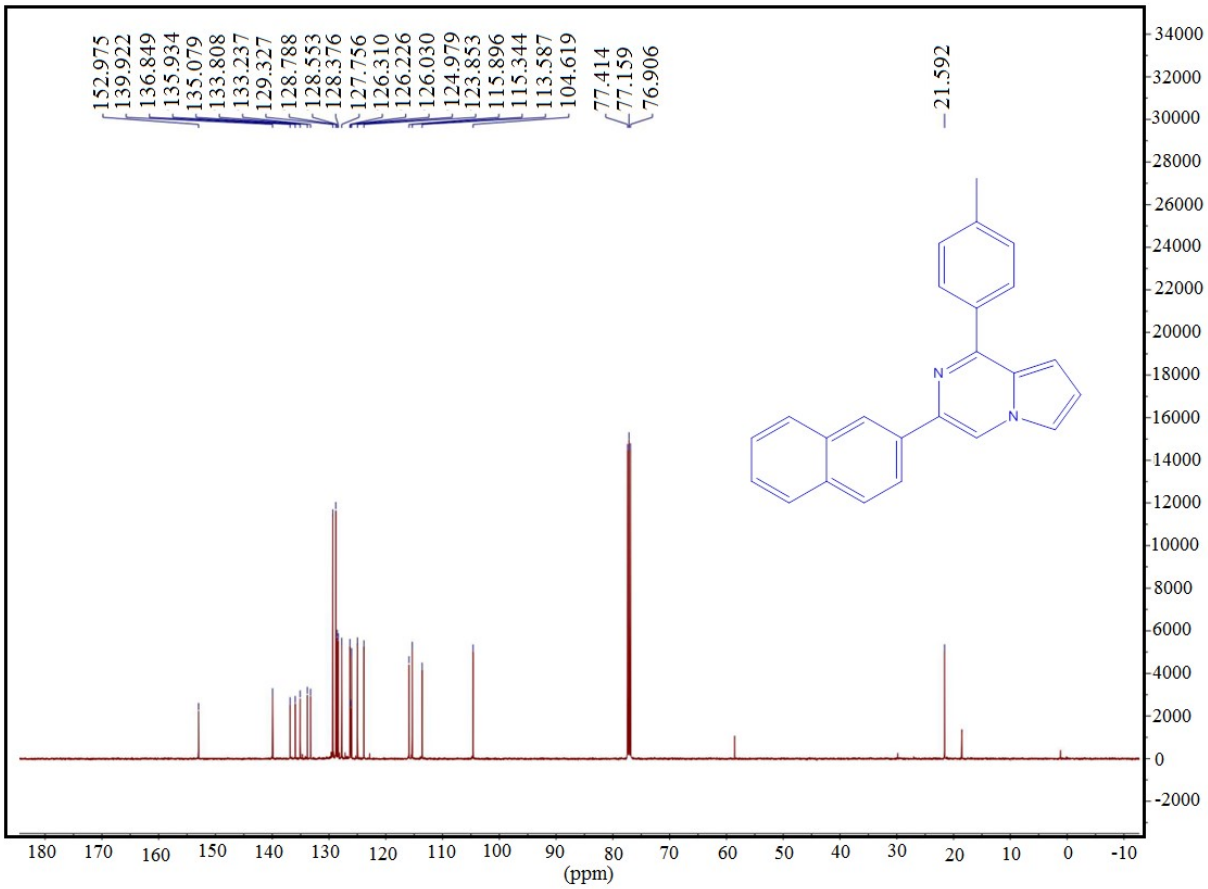
$^{13}C\{^{1}H\}$ NMR Spectrum 3-(furan-2-yl)-1-(p-tolyl)pyrrolo[1,2-a]pyrazine(3a)



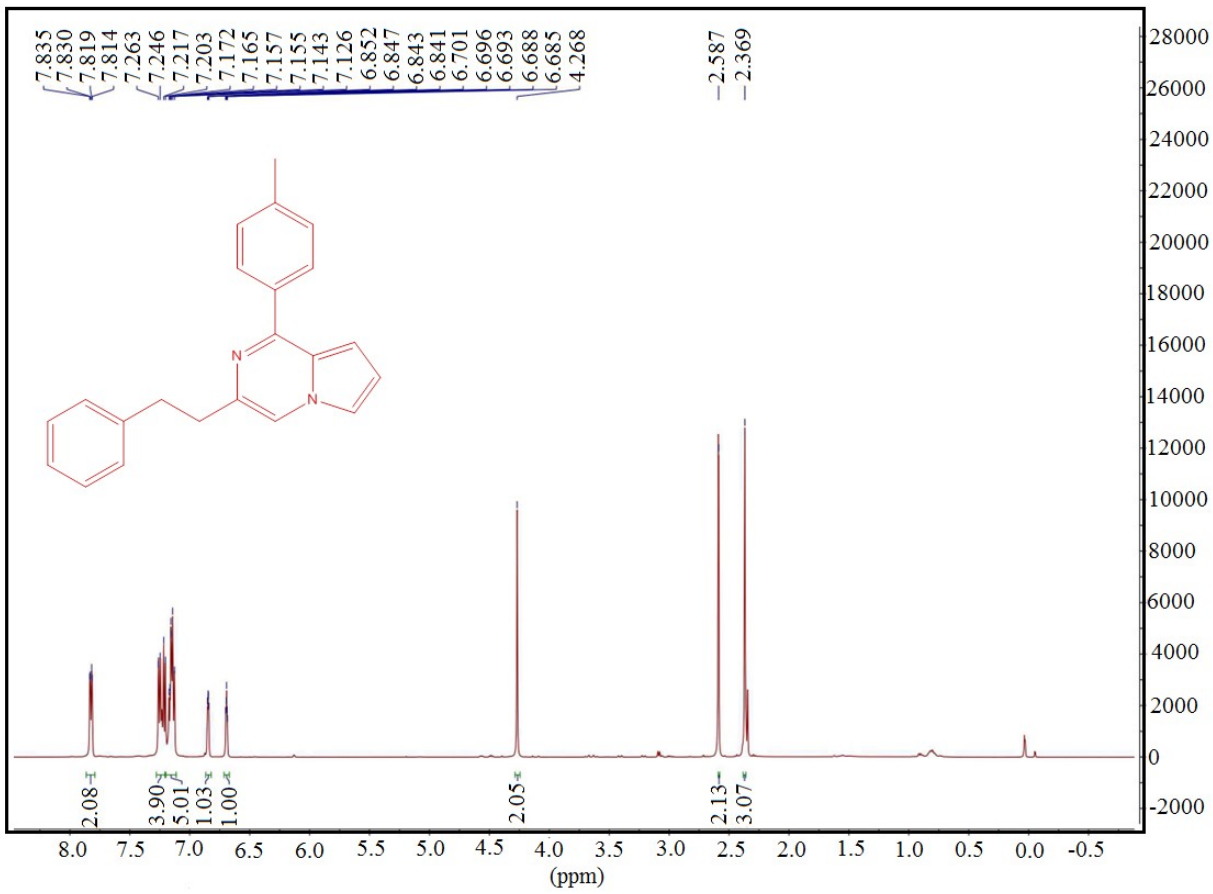
^{1}H NMR Spectrum 3-(naphthalen-2-yl)-1-(*p*-tolyl)pyrrolo[1,2-*a*]pyrazine(3b)



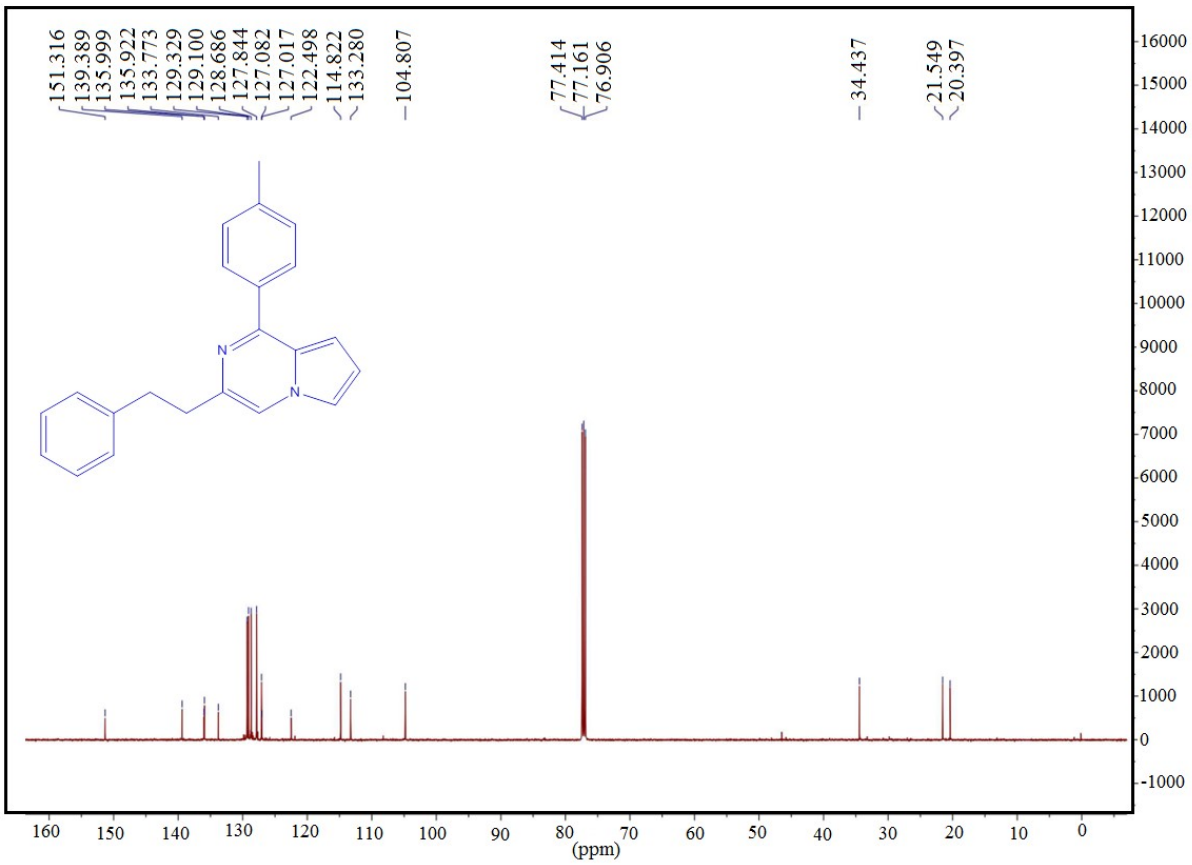
$^{13}C\{^{1}H\}$ NMR Spectrum 3-(naphthalen-2-yl)-1-(*p*-tolyl)pyrrolo[1,2-*a*]pyrazine(3b)



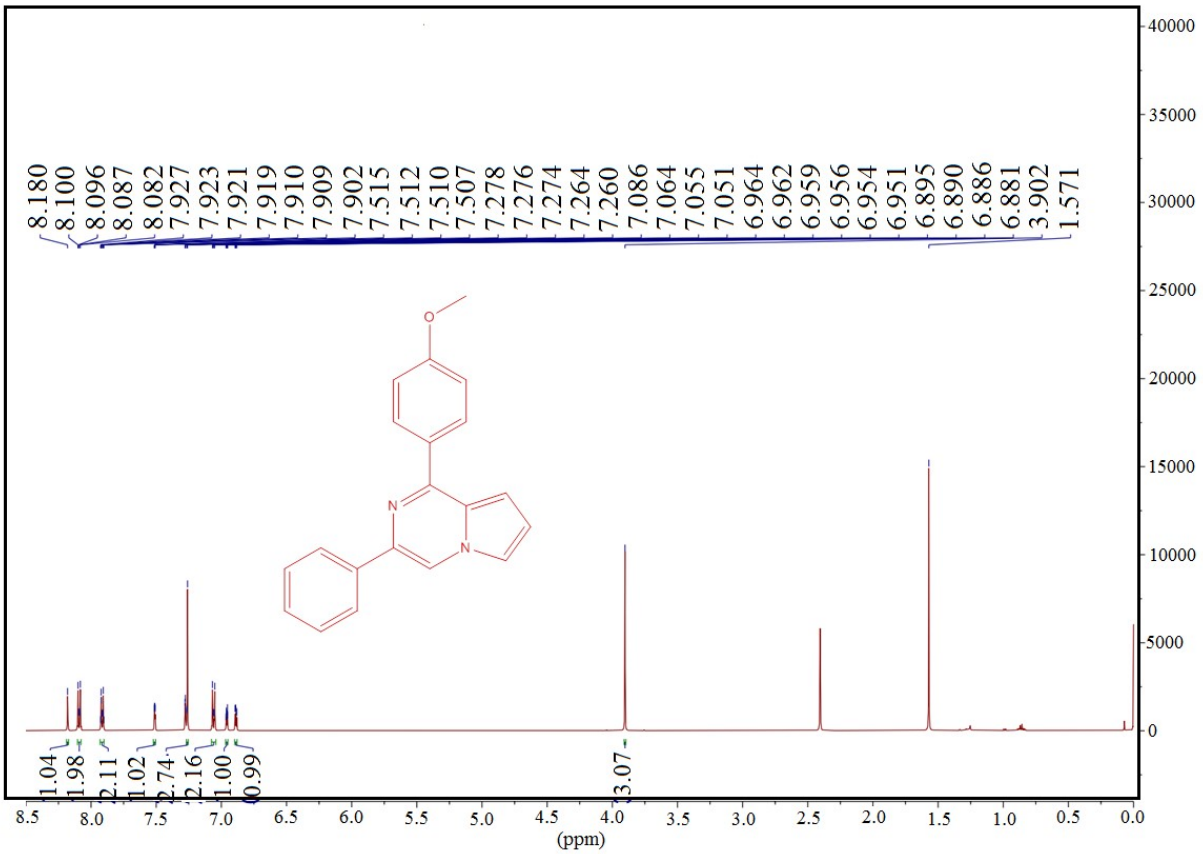
[1]H NMR Spectrum 3-phenethyl-1-(p-tolyl)pyrrolo[1,2-a]pyrazine(3c)



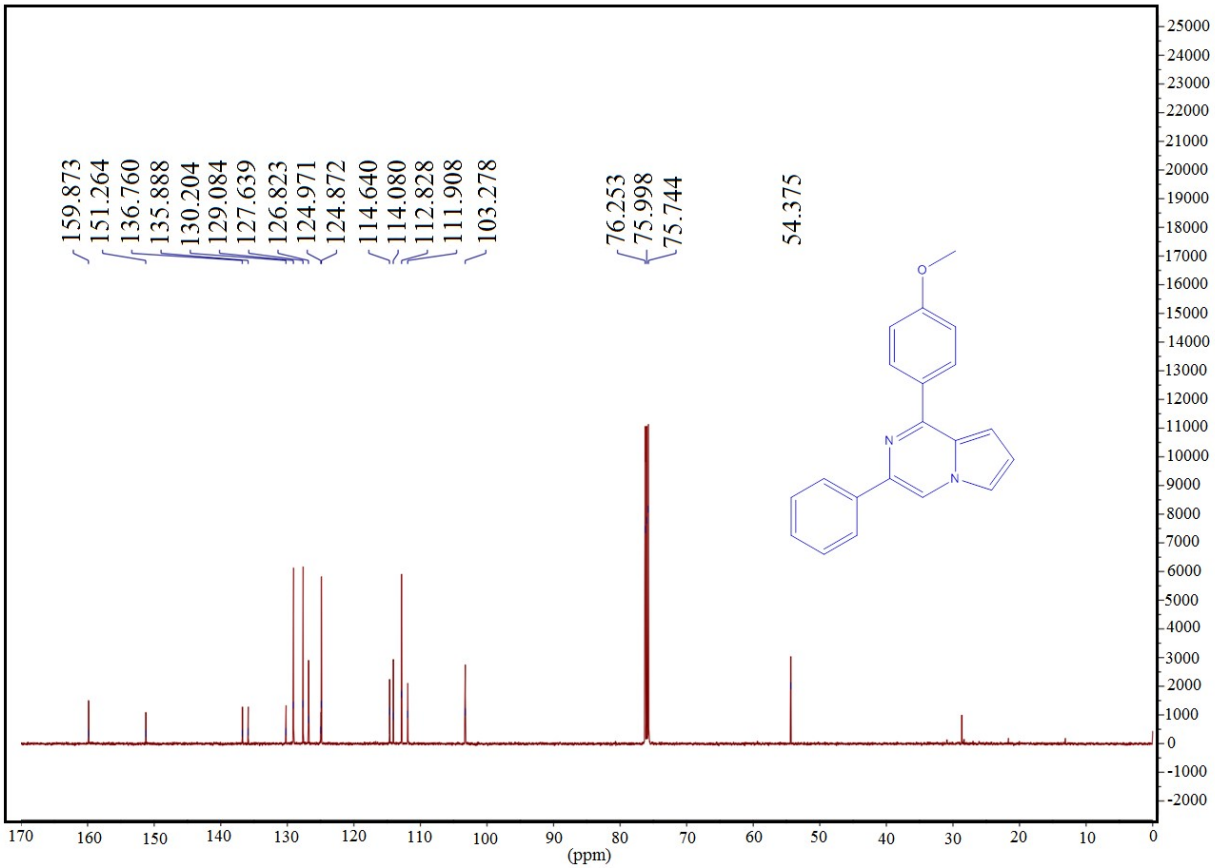
$^{13}C\{^{1}H\}$ NMR Spectrum 3-phenethyl-1-(p-tolyl)pyrrolo[1,2-a]pyrazine(3c)



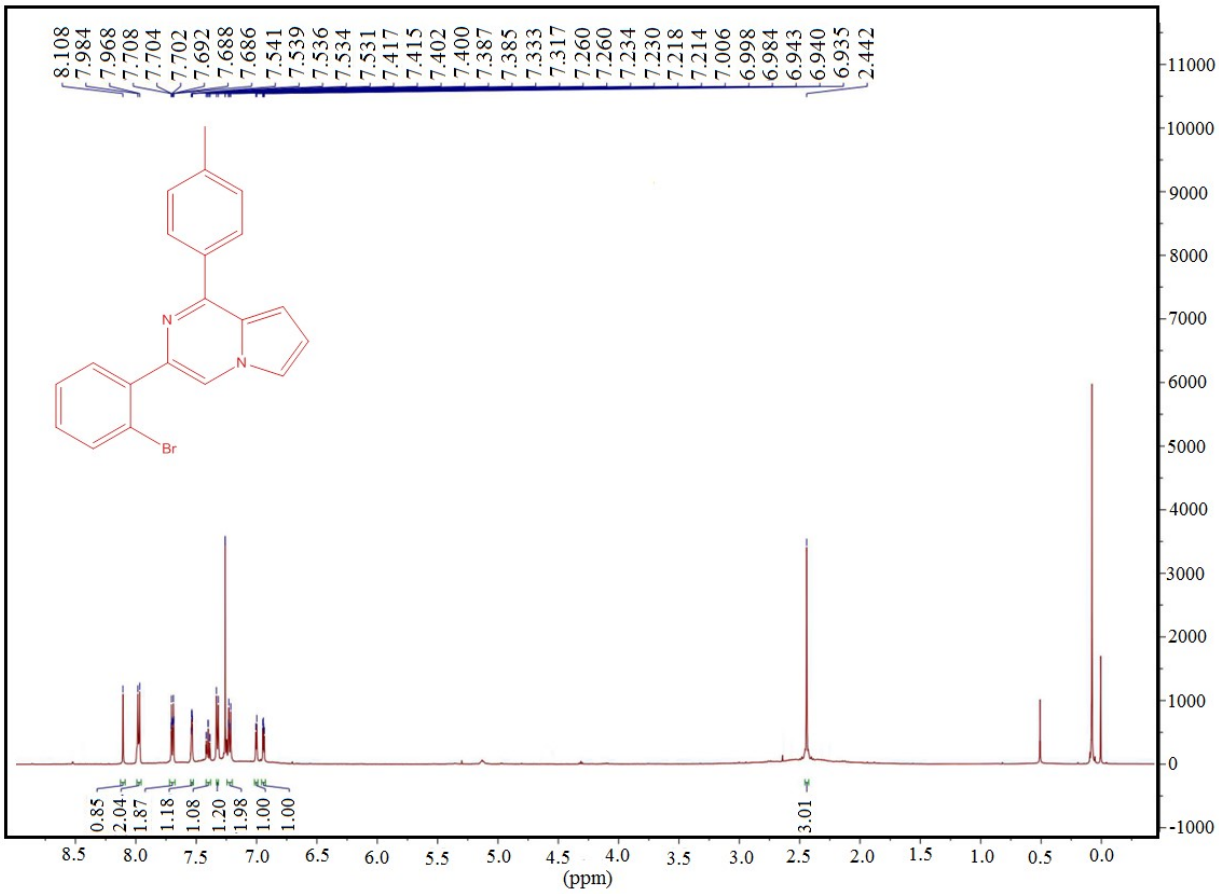
^{1}H NMR Spectrum 1-(4-methoxyphenyl)-3-phenylpyrrolo[1,2-*a*]pyrazine(3d)



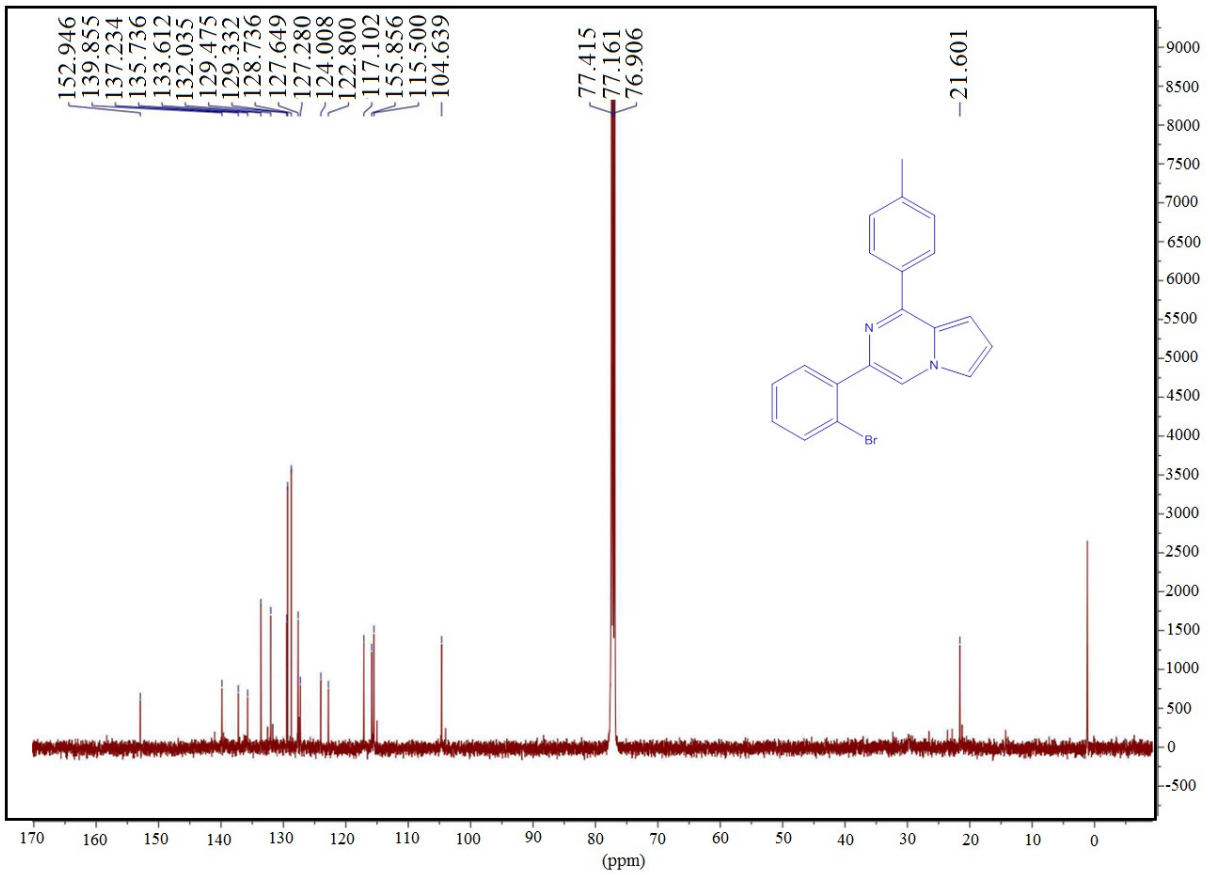
$^{13}C\{^{1}H\}$ NMR Spectrum 1-(4-methoxyphenyl)-3-phenylpyrrolo[1,2-*a*]pyrazine(3d)



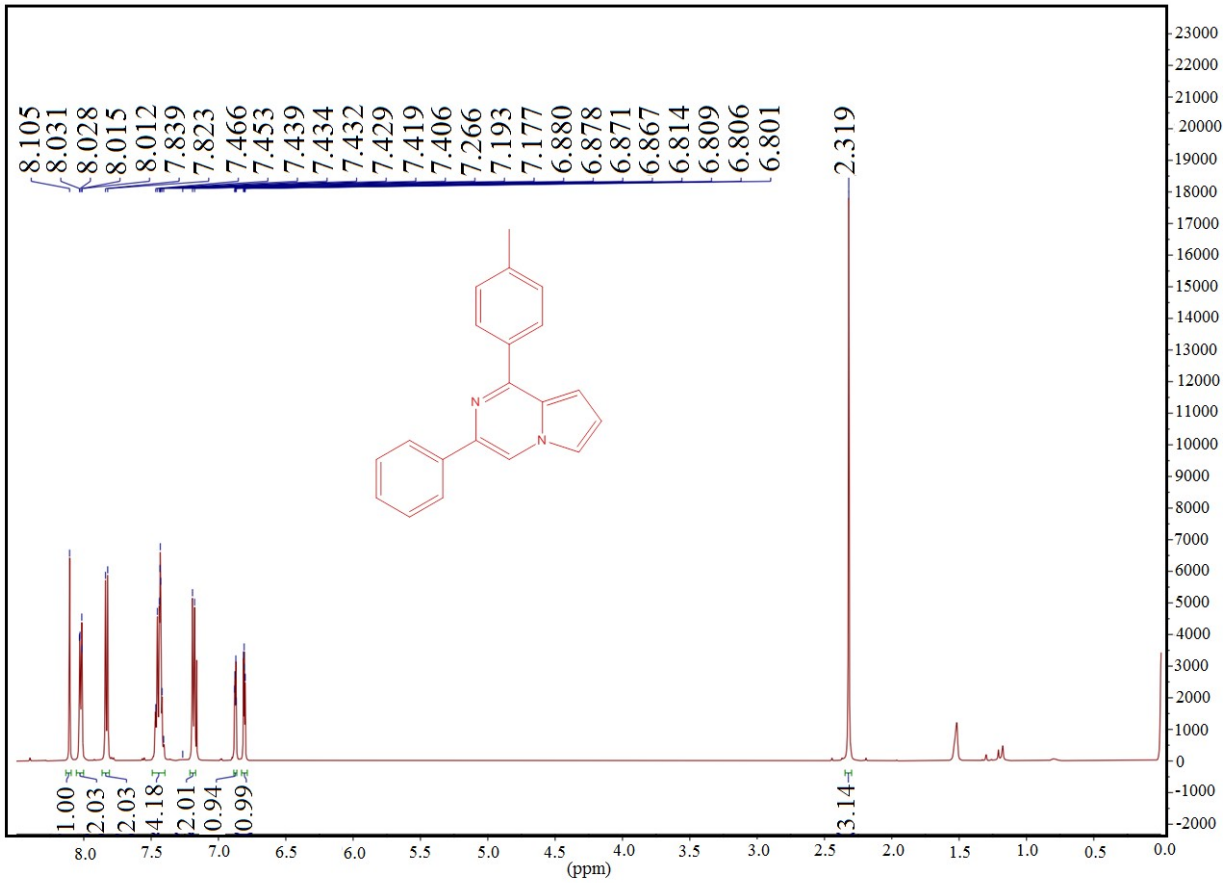
[1]H NMR Spectrum 3-(2-bromophenyl)-1-(*p*-tolyl)pyrrolo[1,2-*a*]pyrazine(3e)



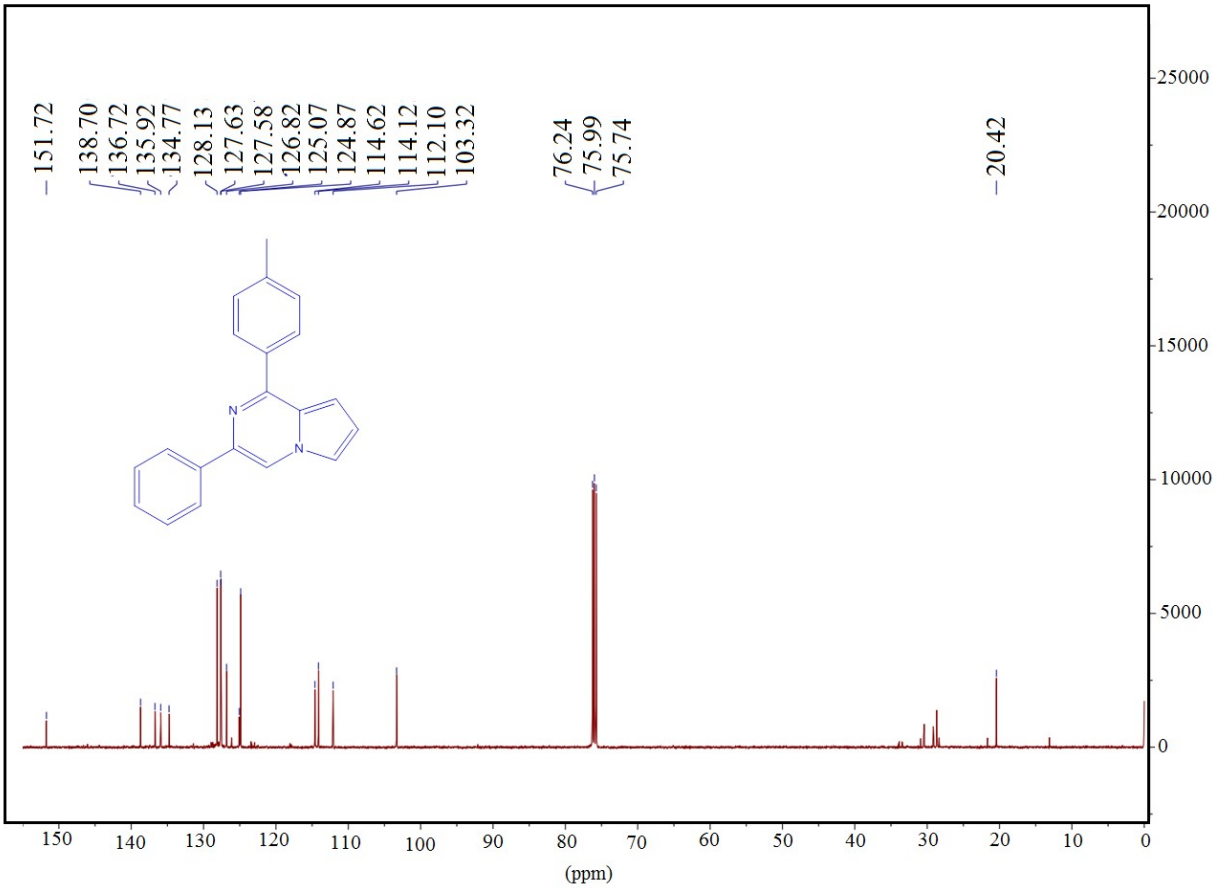
$^{13}C\{^{1}H\}$ NMR Spectrum 3-(2-bromophenyl)-1-(*p*-tolyl)pyrrolo[1,2-*a*]pyrazine(3e)



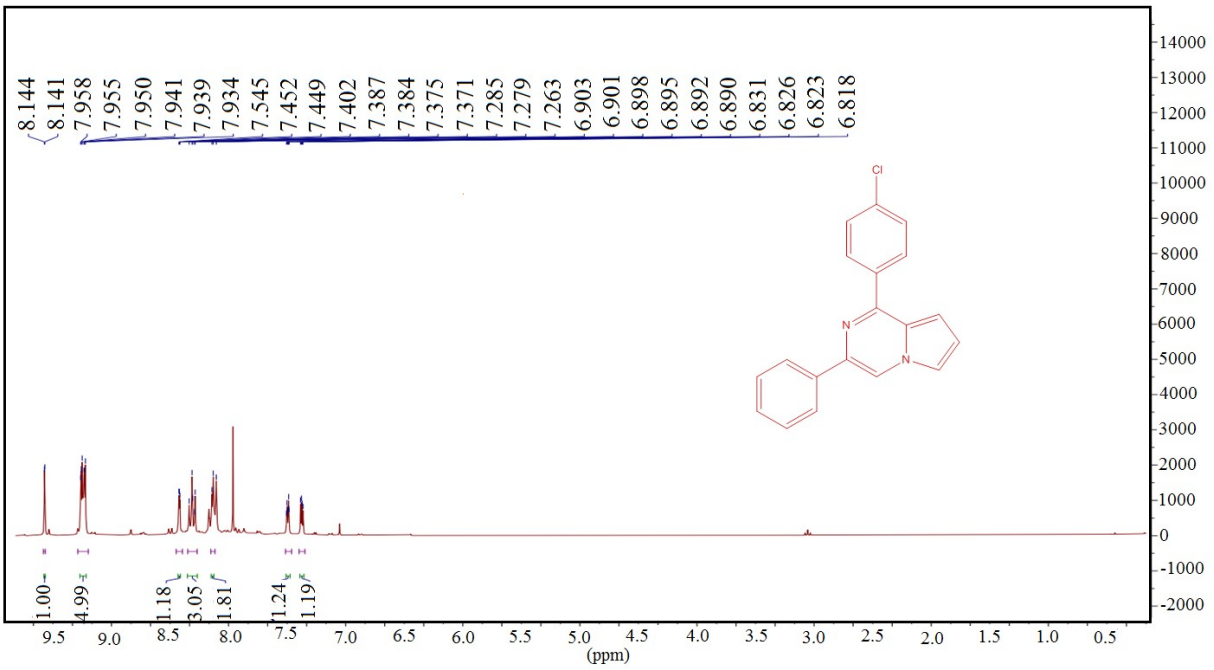
^{1}H NMR Spectrum 3-phenyl-1-(p-tolyl)pyrrolo[1,2-*a*]pyrazine(3f)



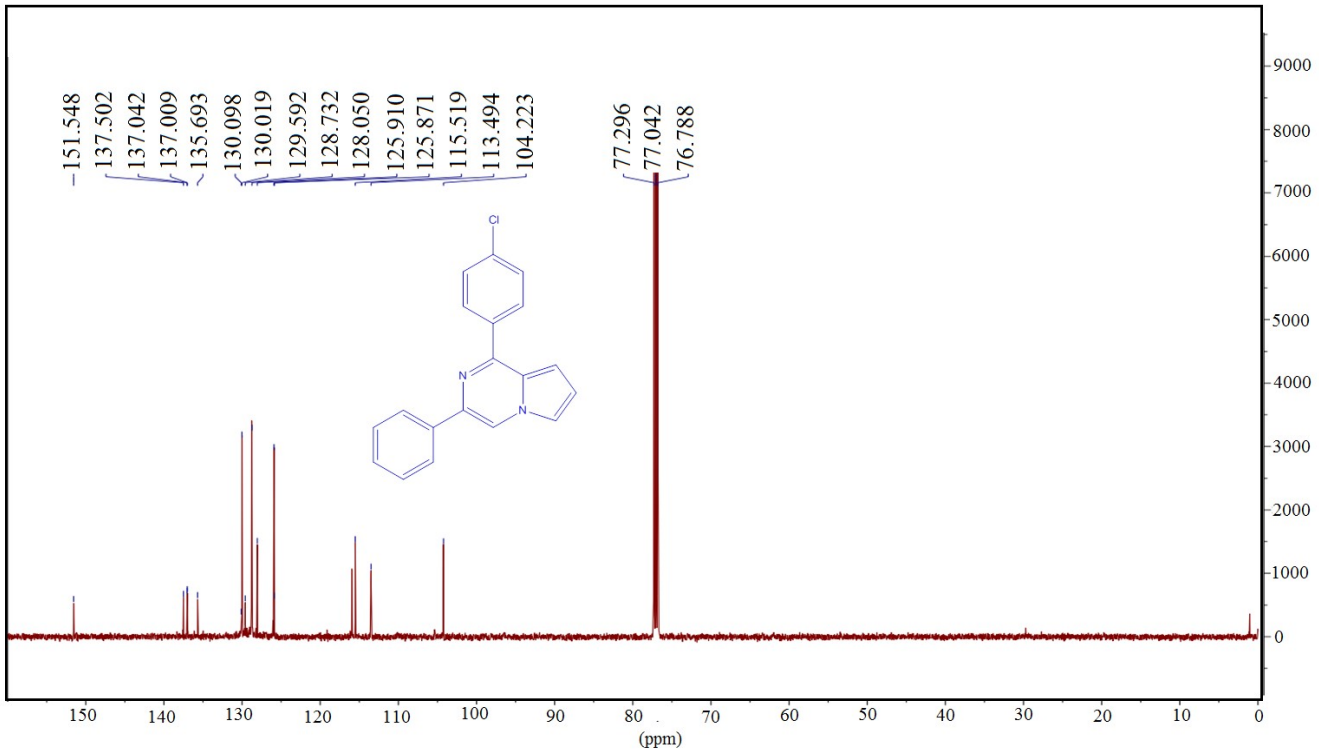
$^{13}C\{^{1}H\}$ NMR Spectrum 3-phenyl-1-(p-tolyl)pyrrolo[1,2-*a*]pyrazine(3f)



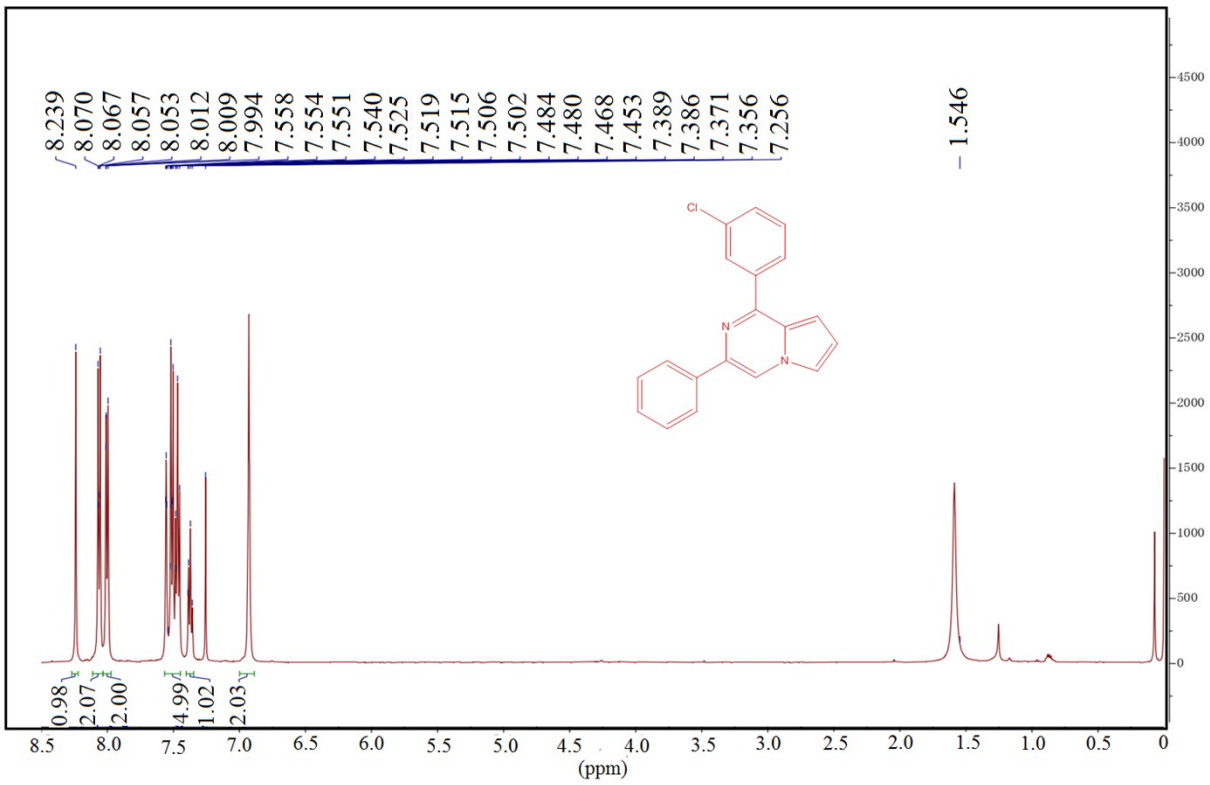
^{1}H NMR Spectrum 1-(4-chlorophenyl)-3-phenylpyrrolo[1,2-*a*]pyrazine(3g)



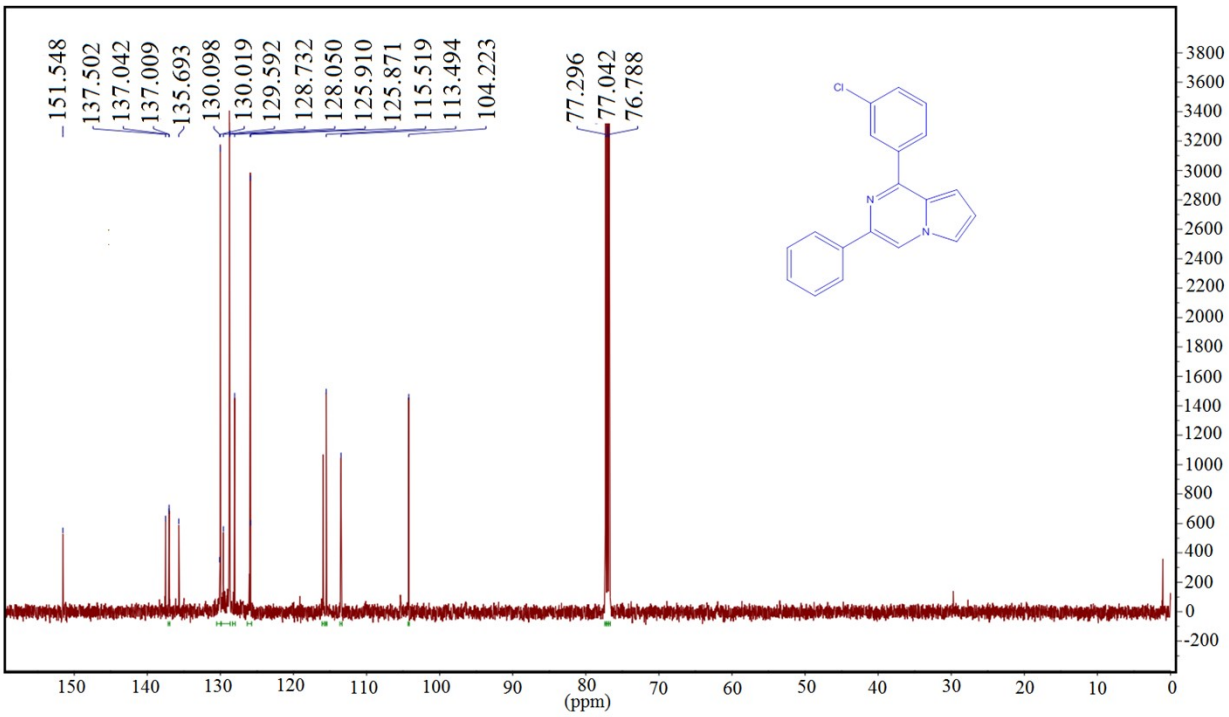
$^{13}C\{^{1}H\}$ NMR Spectrum 1-(4-chlorophenyl)-3-phenylpyrrolo[1,2-*a*]pyrazine(3g)



^{1}H NMR Spectrum 1-(3-chlorophenyl)-3-phenylpyrrolo[1,2-*a*]pyrazine(3h)



^{13}C{^{1}H} NMR Spectrum 1-(3-chlorophenyl)-3-phenylpyrrolo[1,2-*a*]pyrazine(3h)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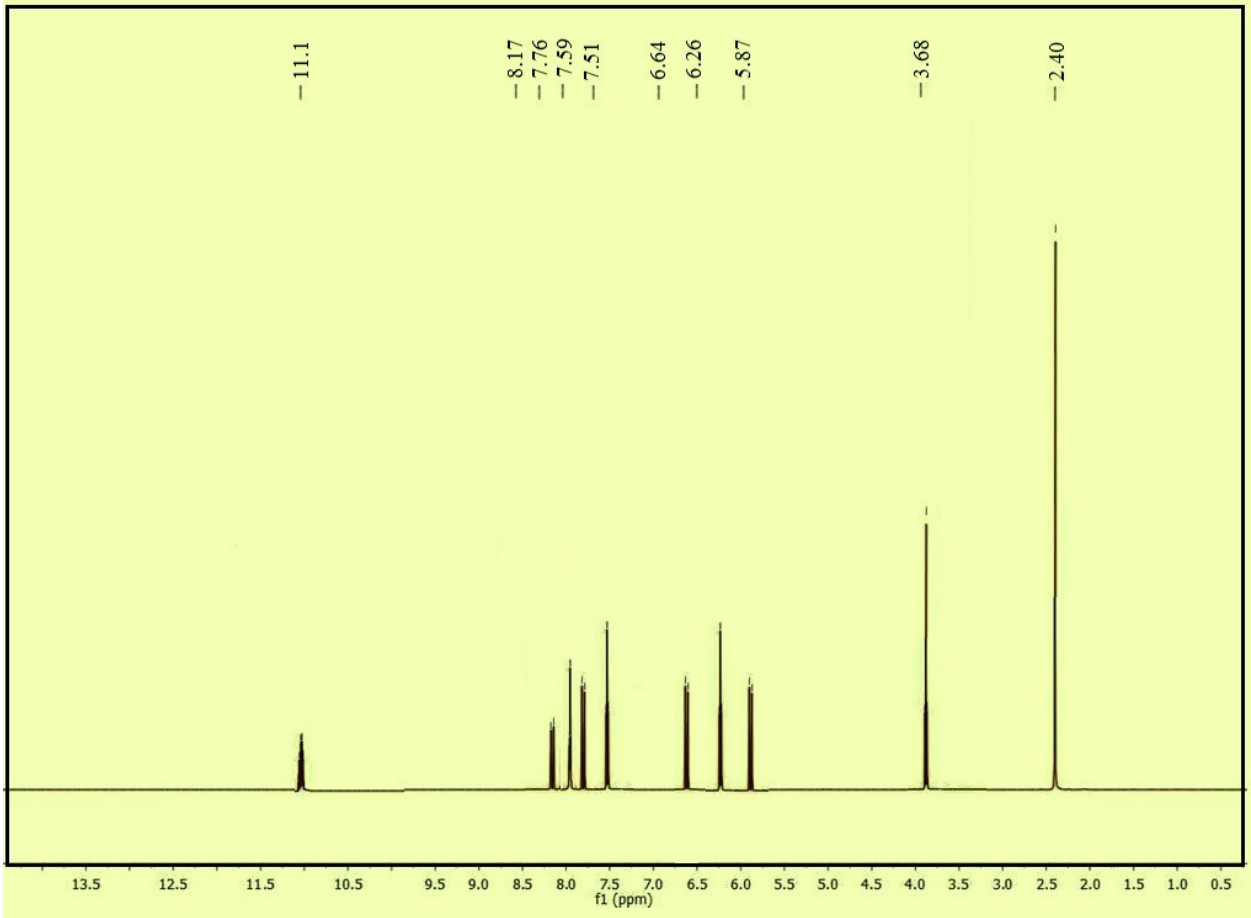
137.042
137.009
135.693
130.098
130.019
129.592
128.732
128.050
125.910
125.871
115.519
113.494
104.223
77.296
77.042
76.788
Cl
N
N
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

^{1}H NMR Solid Spectrum for [Cu(BDC-NH_2)@Schiff-Base-Pd(II)]

The ^{1}HNMR results indicate two types of hydrogen bonded to the amine nitrogen in the structure of the metal-organic framework. This spectrum indicates that the surface amine nitrogens form imine with the ligand in question and are part of free internal amines.



In order to investigate the positive effect of the synthesis and application of this metal organic framework with copper-based catalytic carriers, we synthesized some of them according to the instructions and used them in the synthesis of product number 3a in comparison with the mentioned catalyst. Inputs 1 to 4 can be seen due to the penetration of palladium inside the sites, the available surface of the catalyst is less, as a result, the product efficiency is lower.

Tabel 1. Comparison of the effect of different catalyst carriers containing Cu for use in the synthesis of products with C-N coupling[a].

Entry	Catalyst Carriers	Yield (%)	Refs.
1	Cu-MOF	62	[1]
2	Mn/Cu metal–organic frameworks	51	[2]
3	MOF-891	57	[3]
4	Cu-MOF2	48	[4]
5	[Cu(BDC-NH_2)@Schiff base Pd(II)]catalyst	66	This work

[a]Product sample (3a)

Reference

1. Mollabagher, H., et al., *Cu-metal organic frameworks (Cu-MOF) as an environment-friendly and economical catalyst for one pot synthesis of tacrine derivatives.* RSC advances, 2020. **10**(4): p. 1995-2003.
2. Le, Q.B., et al., *Electrochemical performance of composite electrodes based on rGO, Mn/Cu metal–organic frameworks, and PANI.* Scientific Reports, 2022. **12**(1): p. 664.
3. Nguyen, H.T., et al., *A highly active copper-based metal-organic framework catalyst for a friedel–crafts alkylation in the synthesis of bis (indolyl) methanes under ultrasound irradiation.* Arabian Journal of Chemistry, 2020. **13**(1): p. 1377-1385.
4. Omkaramurthy, B., G. Krishnamurthy, and S. Foro, *Synthesis and characterization of mesoporous crystalline copper metal–organic frameworks for electrochemical energy storage application.* SN Applied Sciences, 2020. **2**: p. 1-14.