

Supporting Information

CuI-Catalyzed Synthesis of Multisubstituted Pyrido[1,2-*a*]pyrimidin-4-ones Through Tandem Ullmann-type C–N Cross-Coupling and Intramolecular Amidation Reaction

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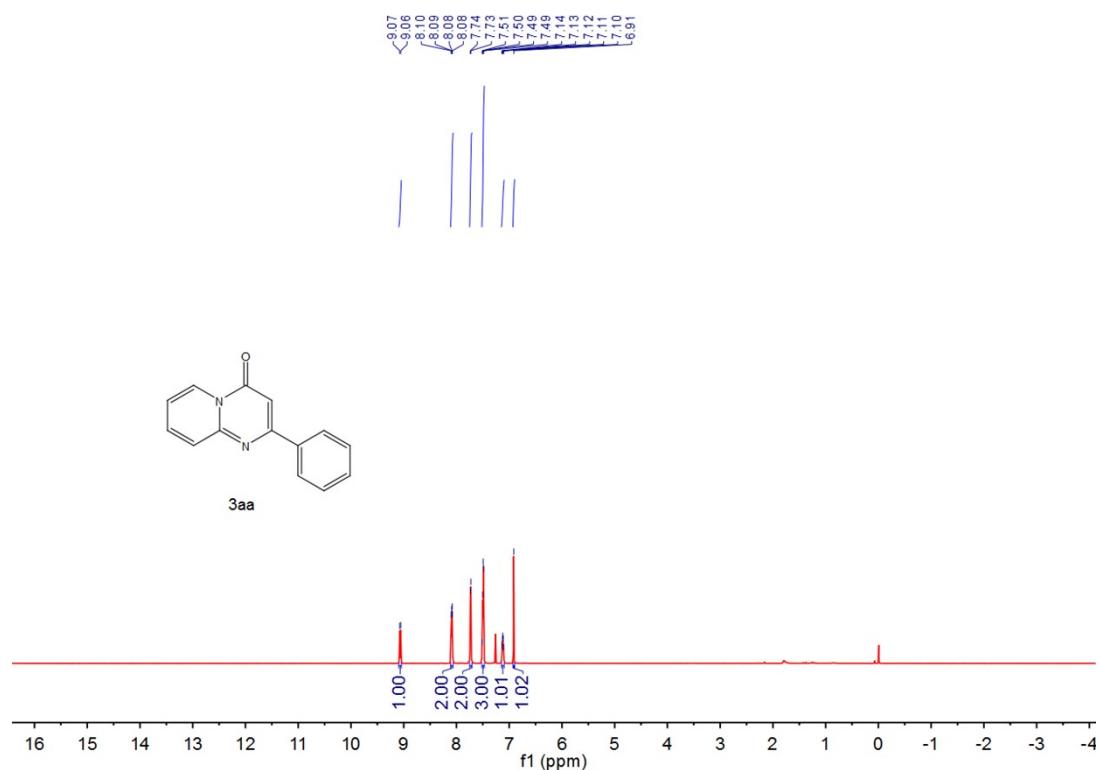
Content

1. Copies of ¹ H NMR and ¹³ C NMR spectra of the products	S-2
2. High-resolution mass spectra of new compounds.....	S-27
3. IR spectra of new compounds.....	S-29

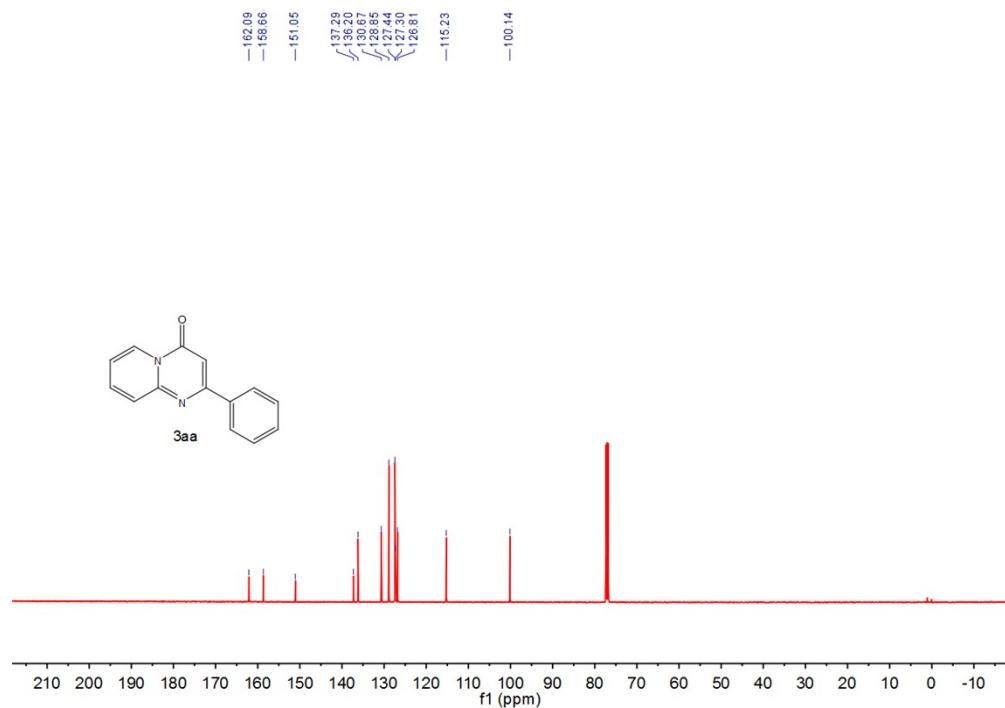
1. Copies of ^1H NMR and ^{13}C NMR spectra of the products

2-*Phenyl-4H-pyrido[1,2-a]pyrimidin-4-one*(3aa)

^1H spectrum of 3aa

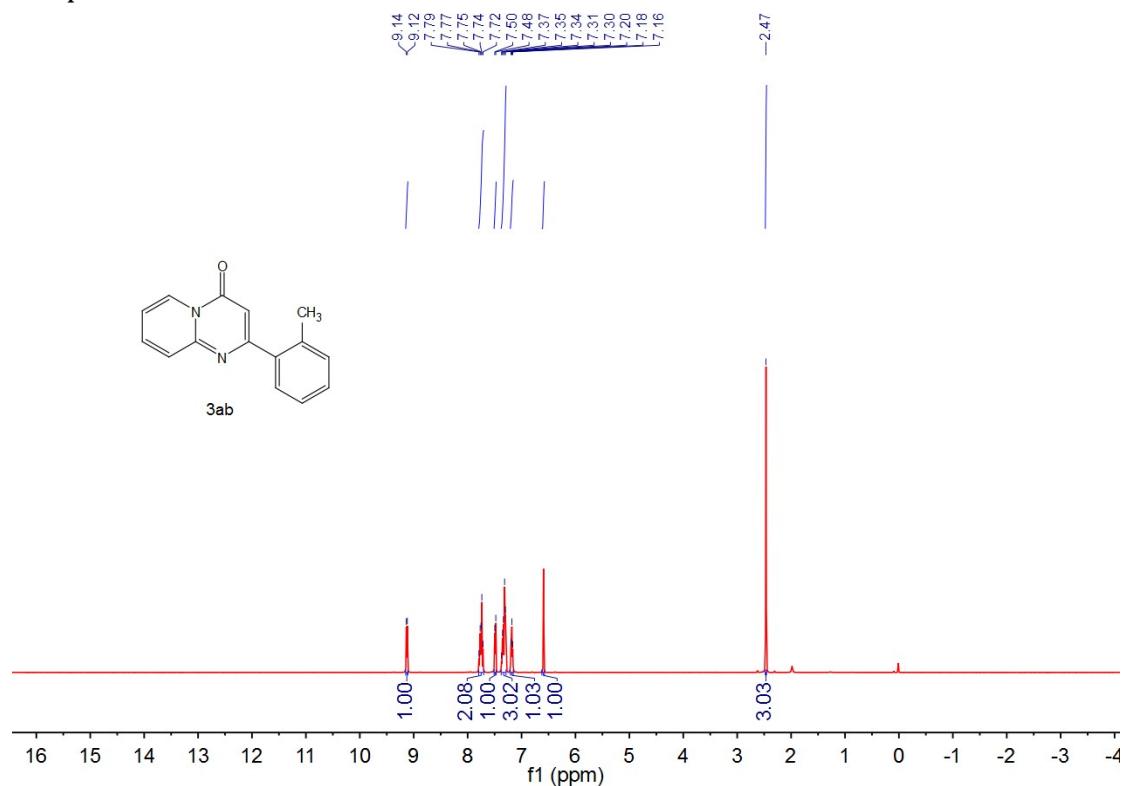


^{13}C spectrum of 3aa

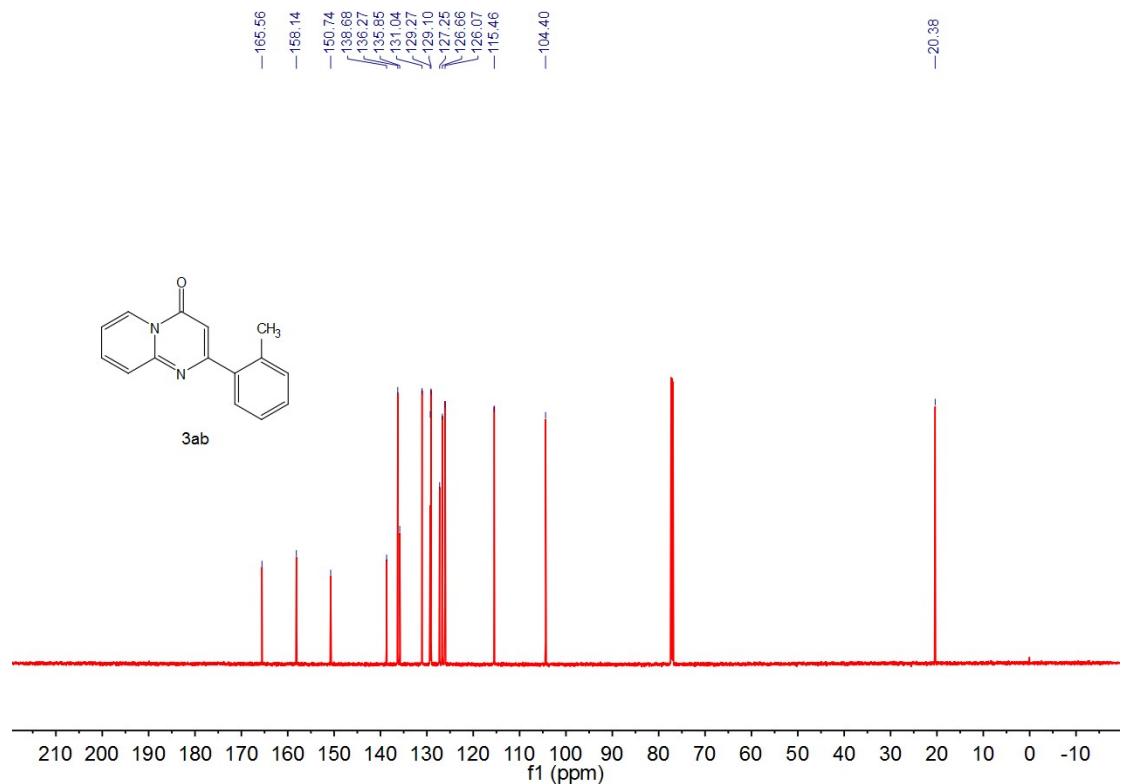


2-(*o-tolyl*)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(3ab)

¹H spectrum of **3ab**

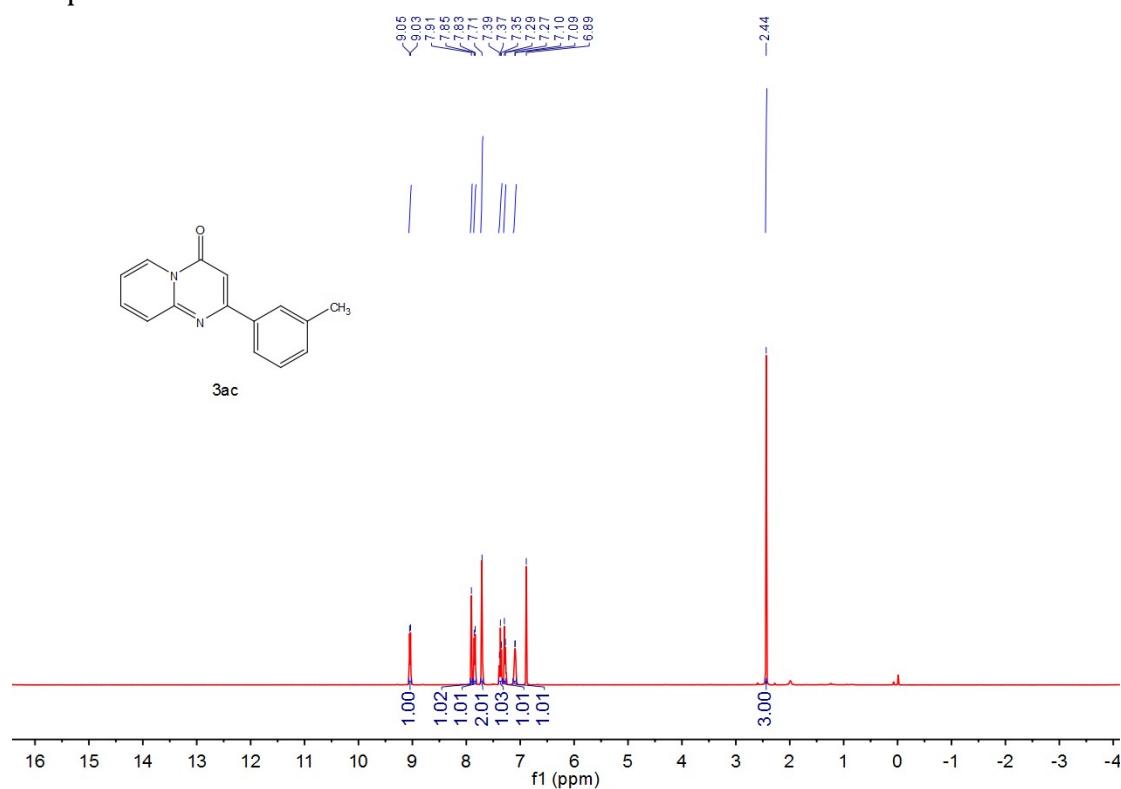


¹³C spectrum of **3ab**

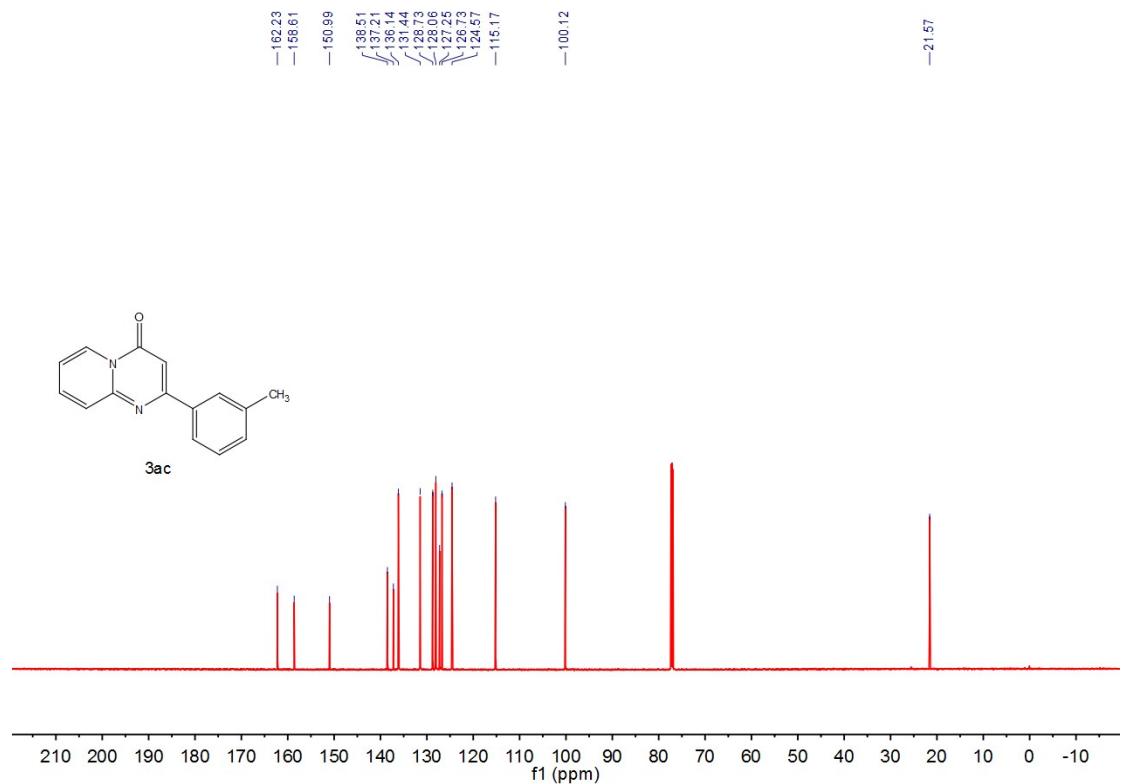


*2-(*m*-tolyl)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(**3ac**)*

¹H spectrum of 3ac

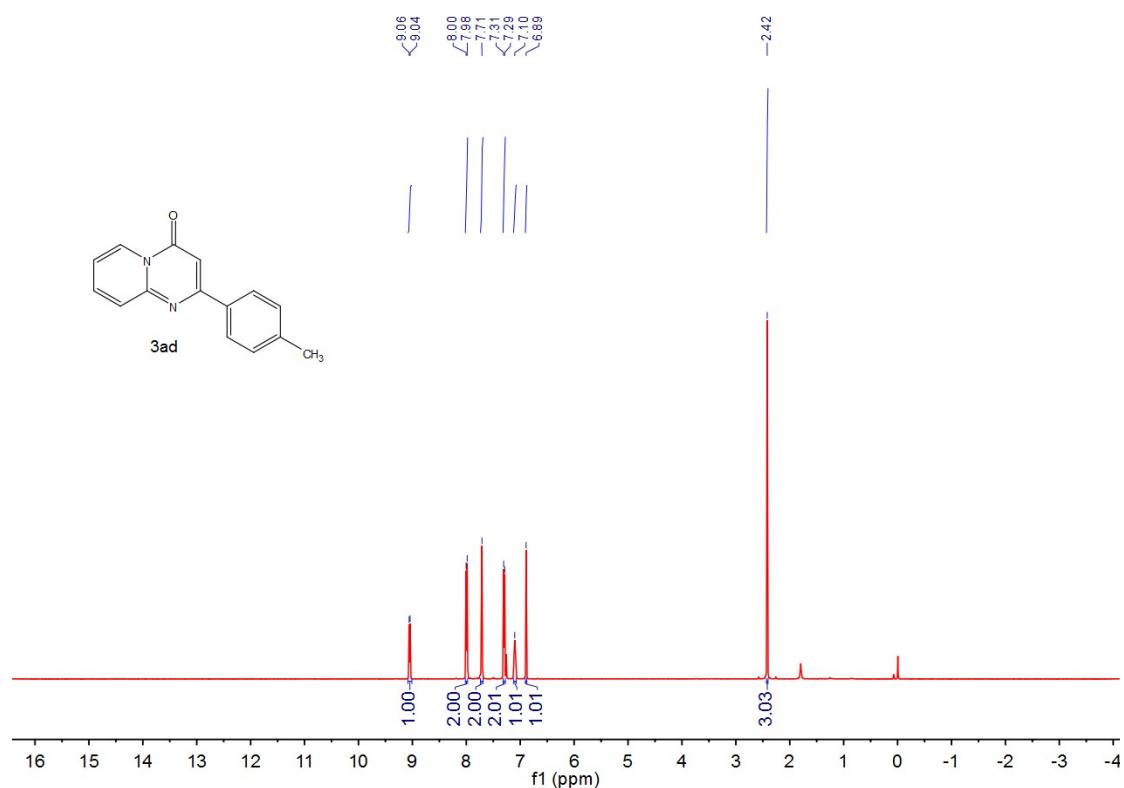


¹³C spectrum of 3ac

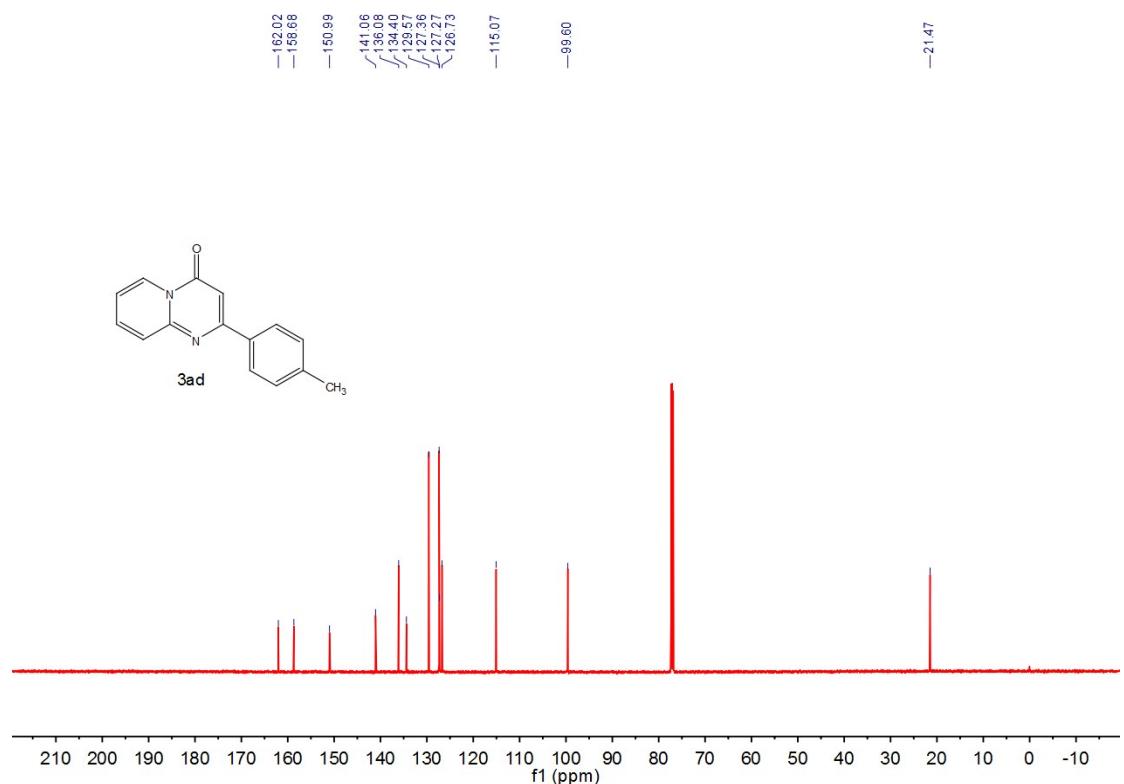


2-(*p*-tolyl)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(3ad)

¹H spectrum of **3ad**

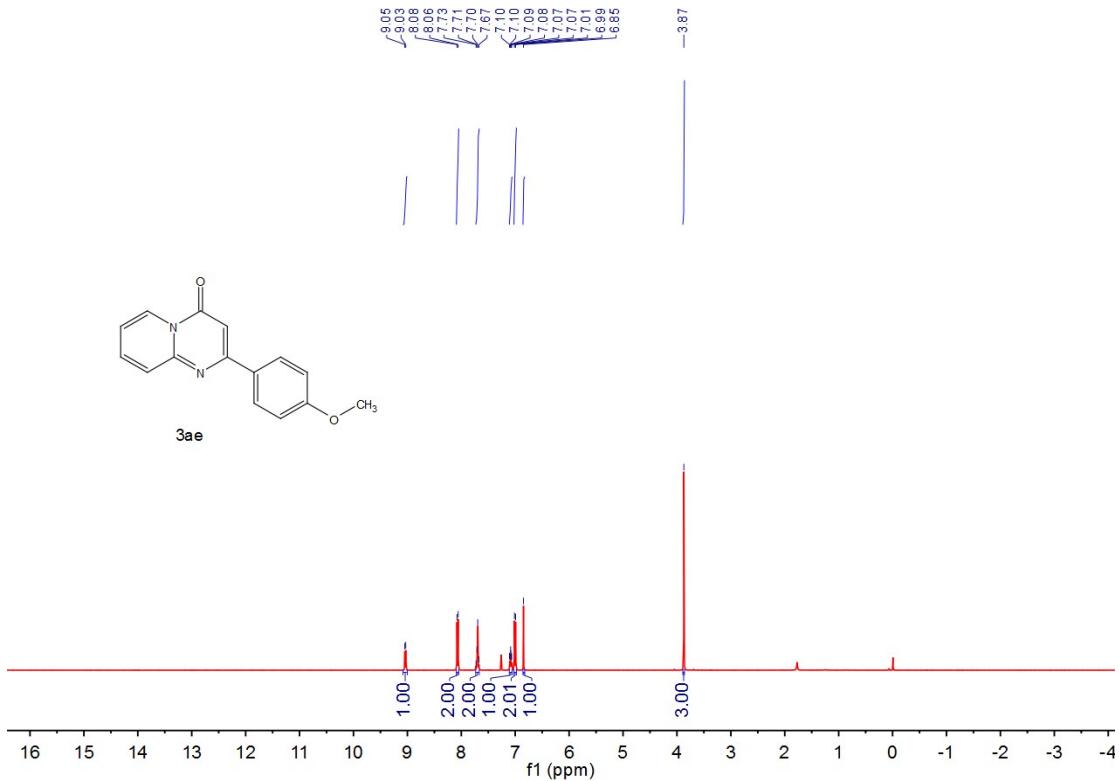


¹³C spectrum of **3ad**

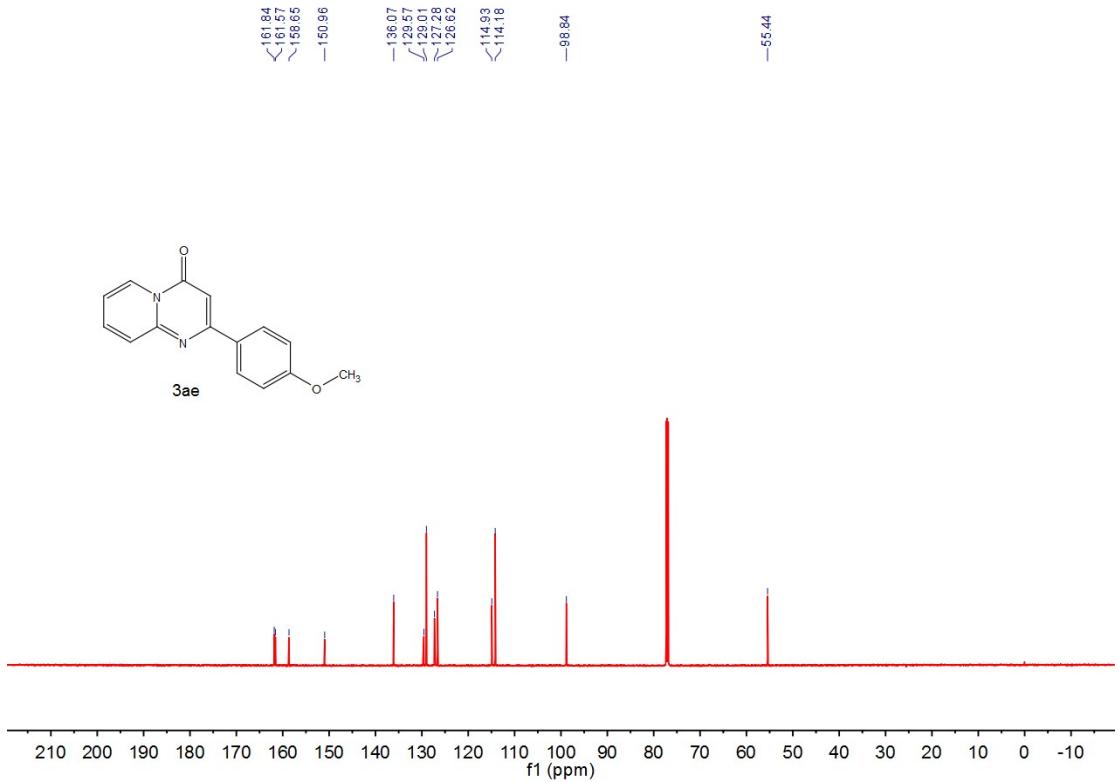


*2-(4-Methoxyphenyl)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(**3ae**)*

¹H spectrum of **3ae**

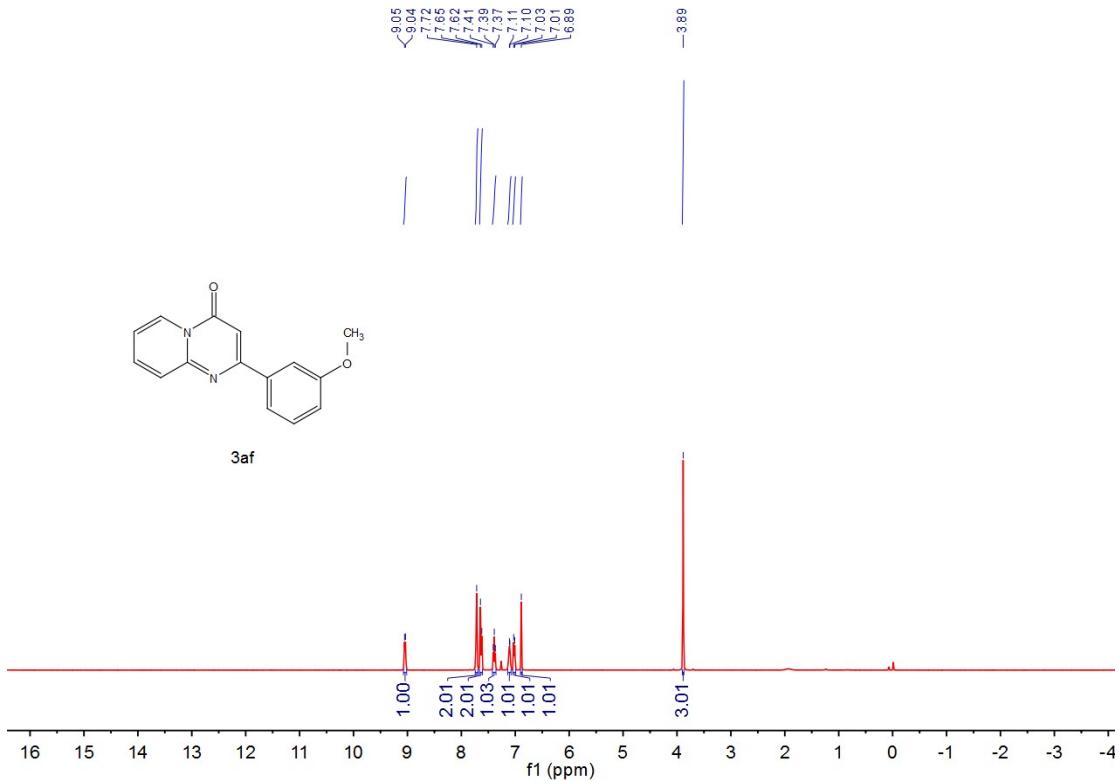


^{13}C spectrum of 3ae

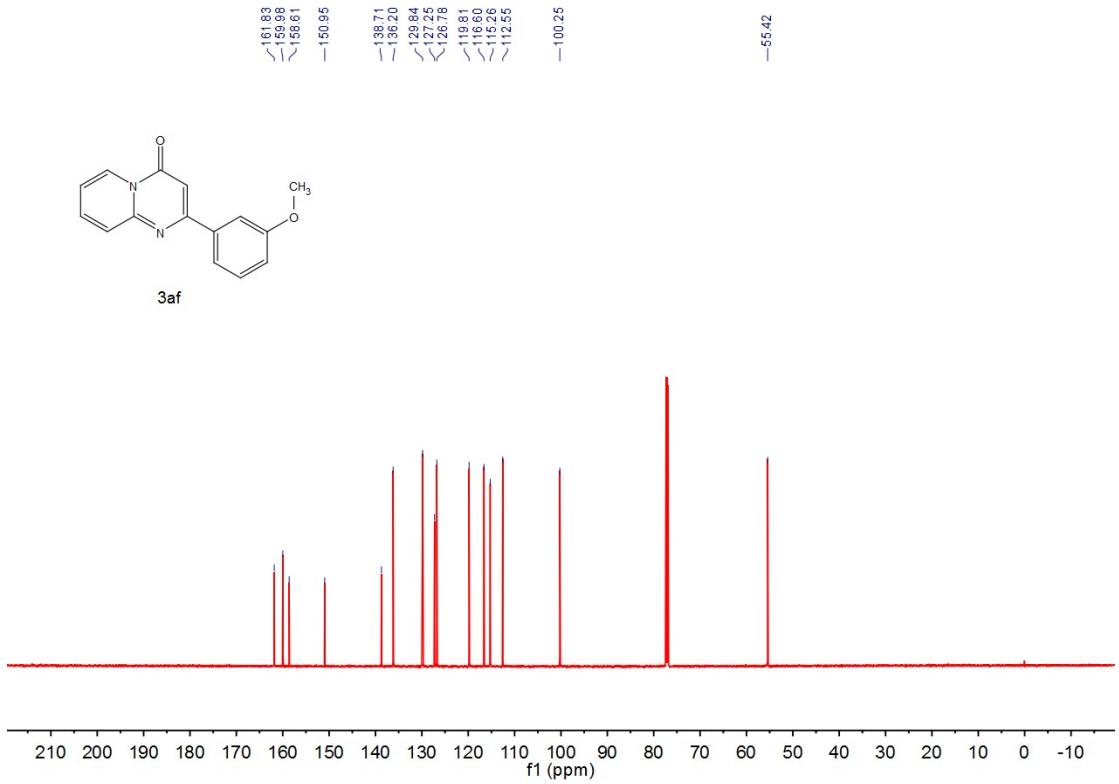


2-(3-Methoxyphenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3af)

^1H spectrum of 3af

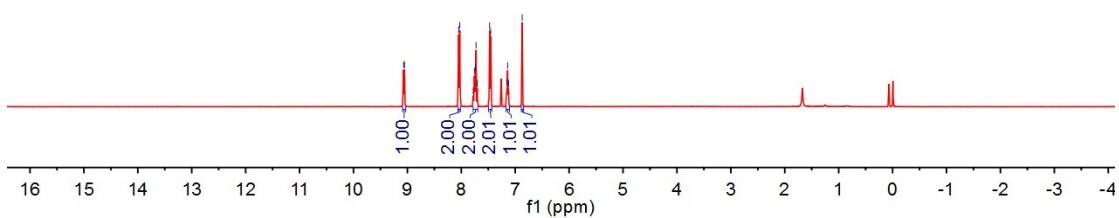
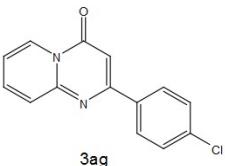
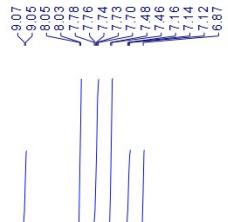


^{13}C spectrum of **3af**



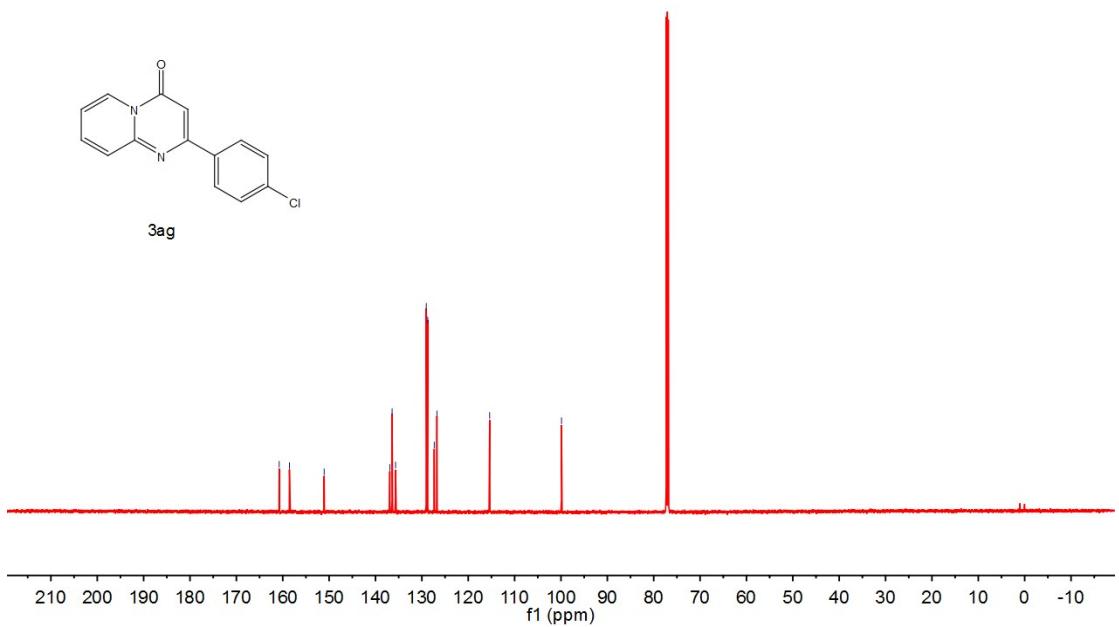
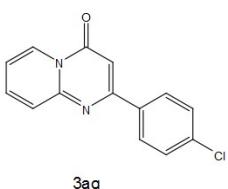
2-(4-Chlorophenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(**3ag**)

^1H spectrum of **3ag**



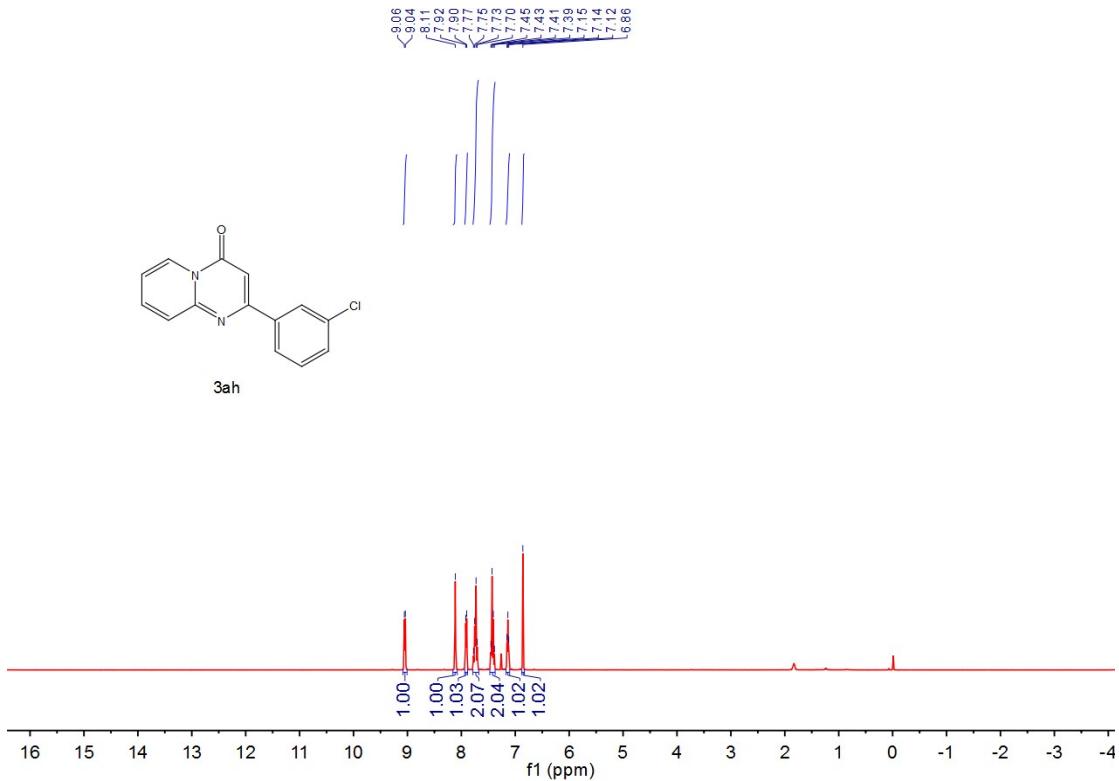
¹³C spectrum of 3ag

160.76
~158.56
—153.07
136.91
~136.41
~136.67
~129.05
~128.74
~127.33
~126.75
—115.38
—99.88

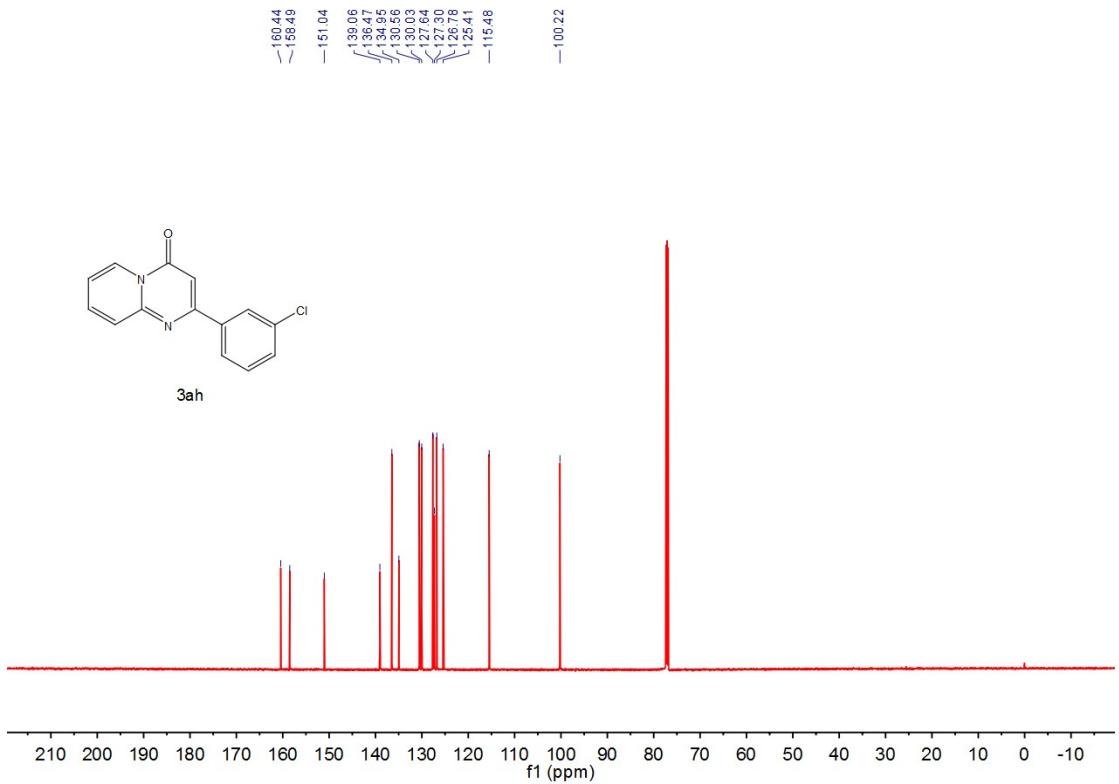


2-(3-Chlorophenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3ah)

¹H spectrum of 3ah

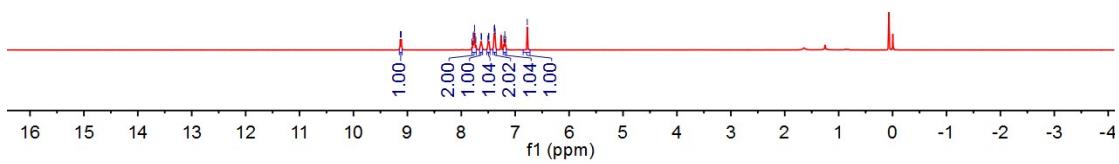
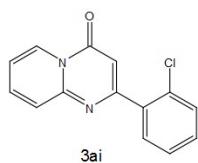
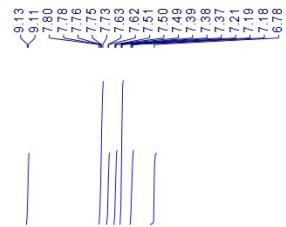


¹³C spectrum of **3ah**



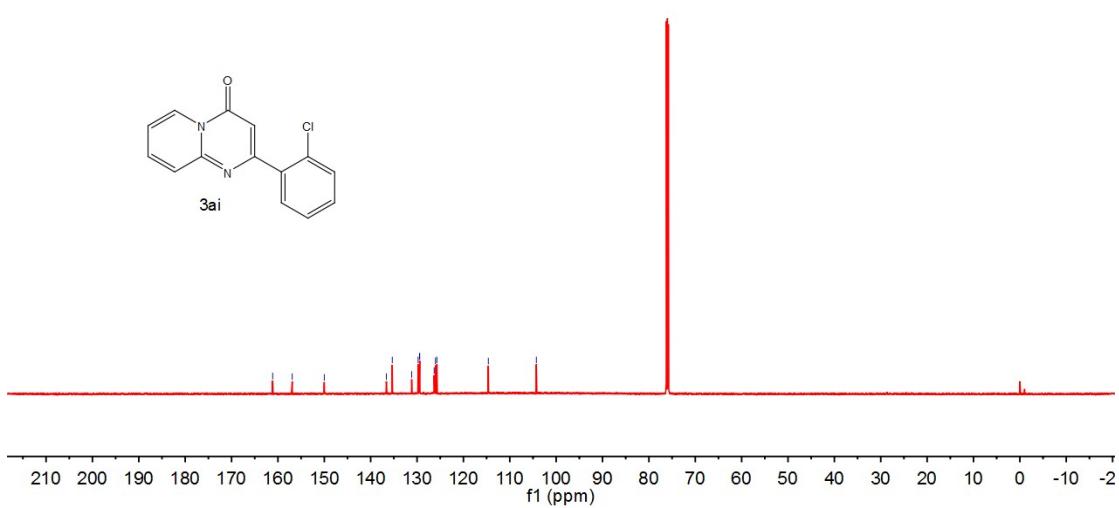
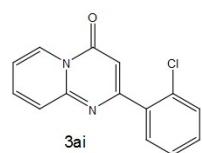
2-(2-Chlorophenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3ai)

¹H spectrum of **3ai**



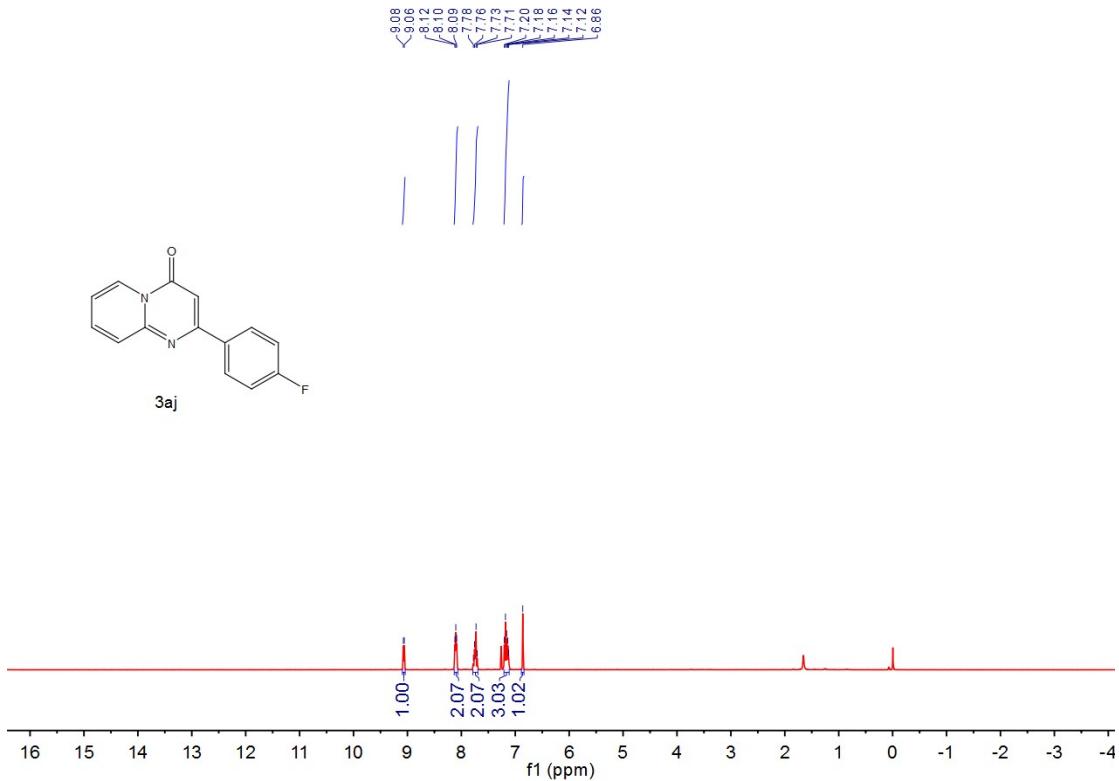
¹³C spectrum of 3ai

—161.14
—156.92
—156.01
—156.61
—136.61
—135.34
—131.15
—127.77
—124.42
—124.44
—123.32
—125.03
—125.72
—114.63
—104.27

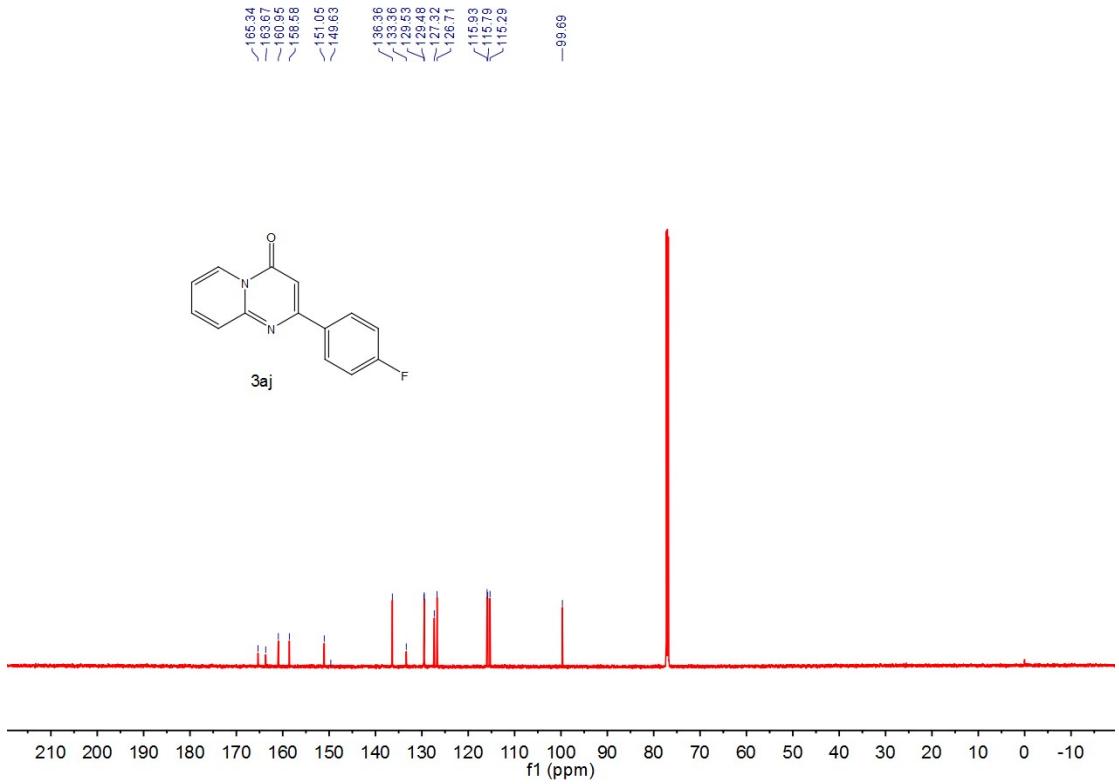


2-(4-Fluorophenyl)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(3aj)

¹H spectrum of 3aj

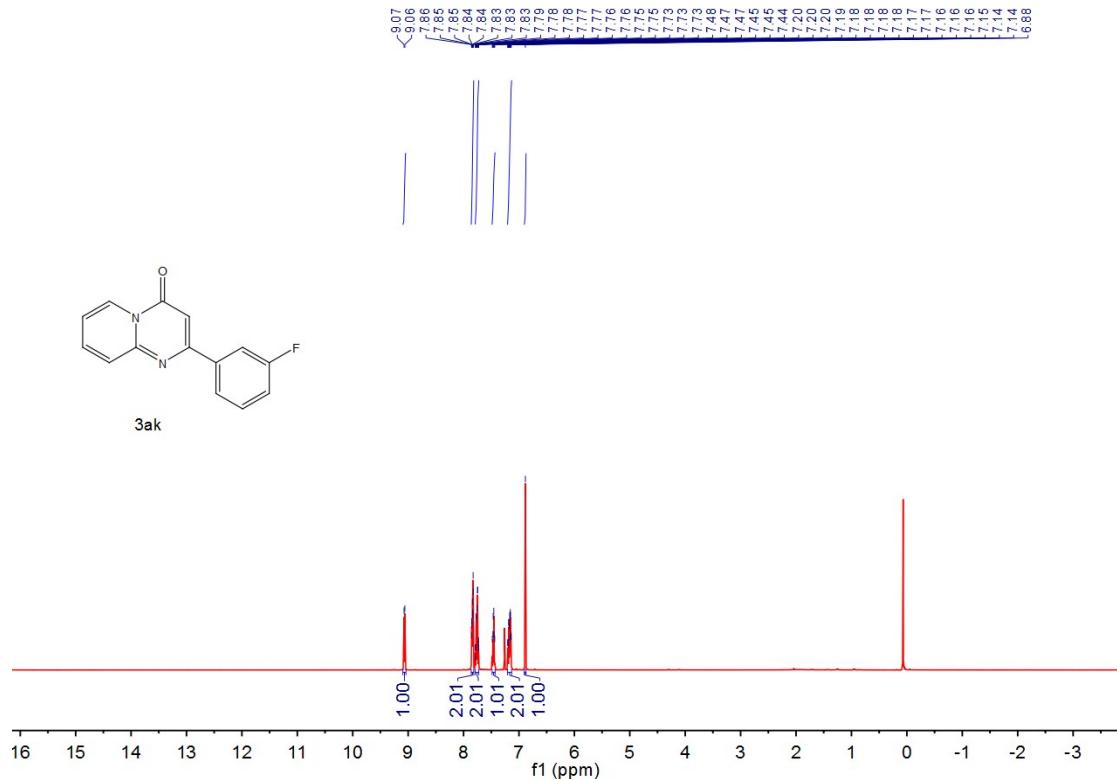


¹³C spectrum of **3aj**



2-(3-Fluorophenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3ak)

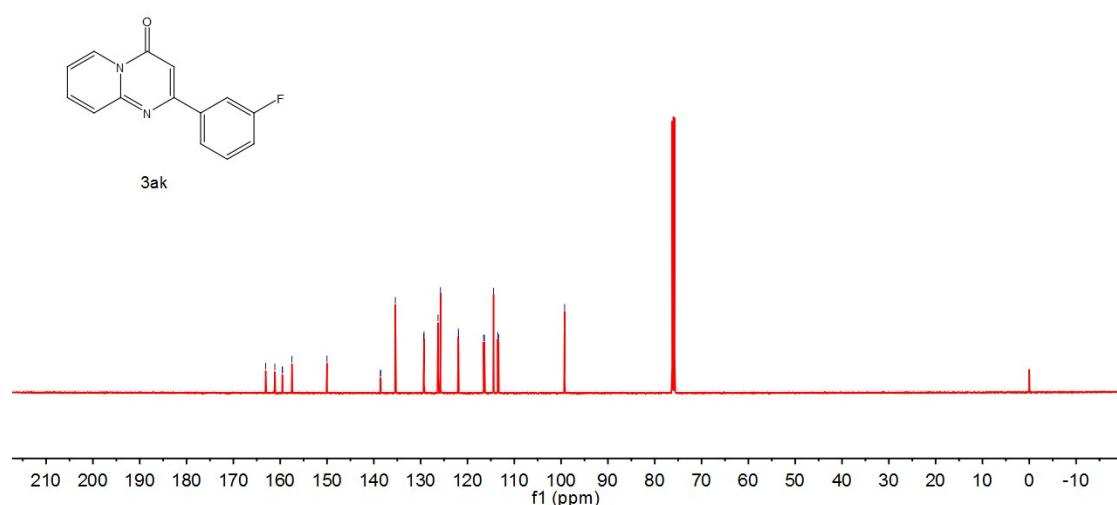
¹H spectrum of **3ak**



¹³C spectrum of **3ak**

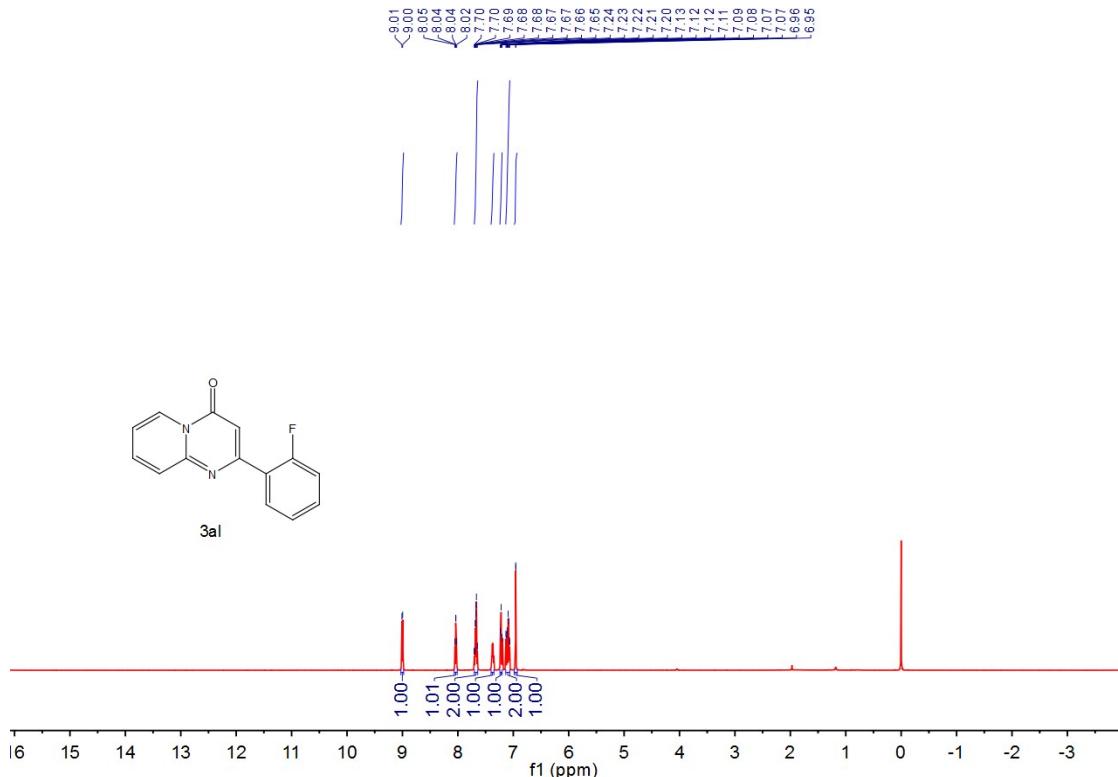


A list of carbon chemical shifts (¹³C NMR) for compound **3ak** in ppm: 163.11, 161.15, 159.54, 159.52, 157.52, 150.01, 139.59, 139.53, 139.41, 129.34, 129.27, 125.96, 125.29, 121.93, 121.91, 116.56, 116.38, 114.43, 113.54, 113.35, -99.25.

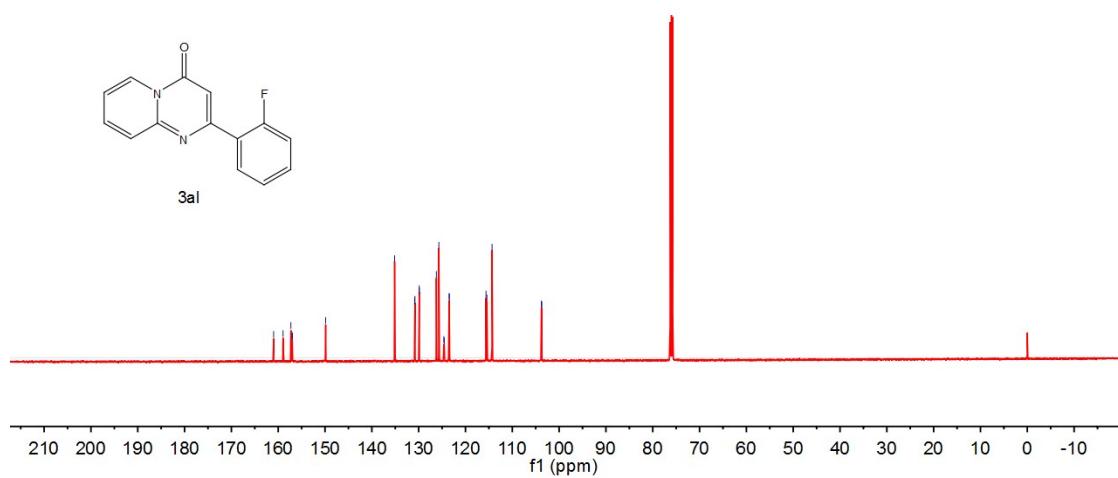
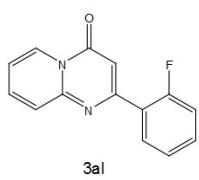


2-(2-Fluorophenyl)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(**3al**)

¹H spectrum of **3al**

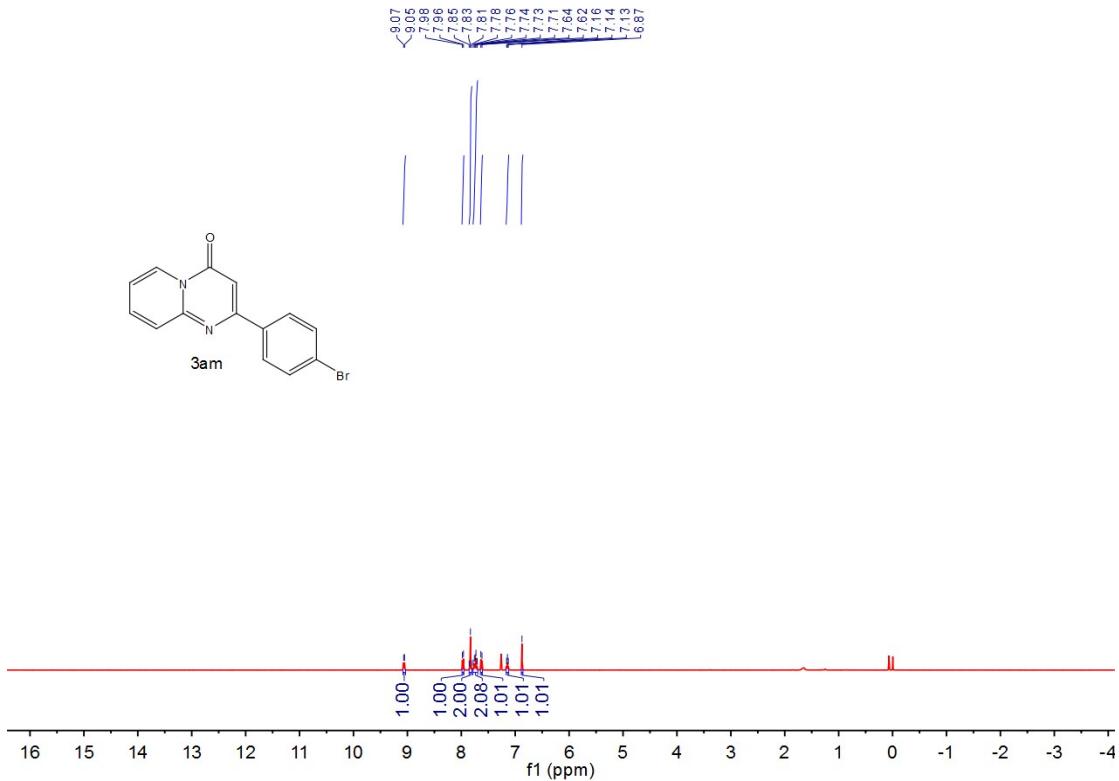


¹³C spectrum of 3al

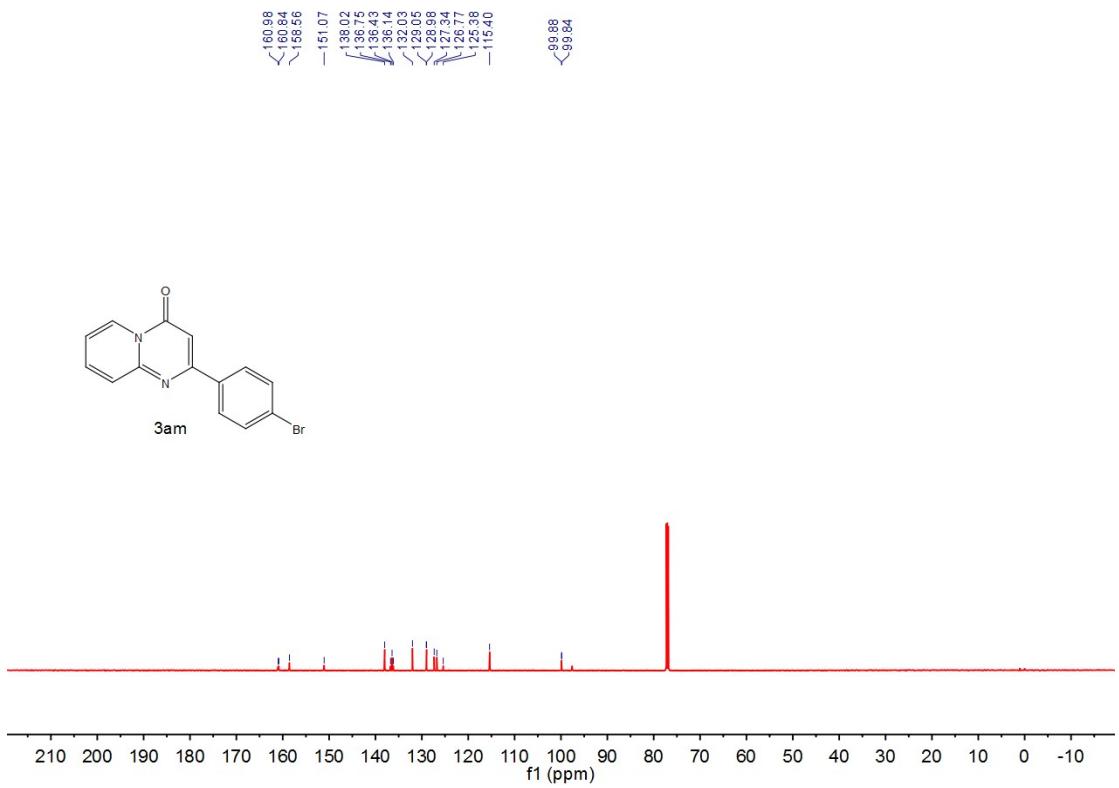


2-(4-Bromophenyl)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(3am)

¹H spectrum of 3am

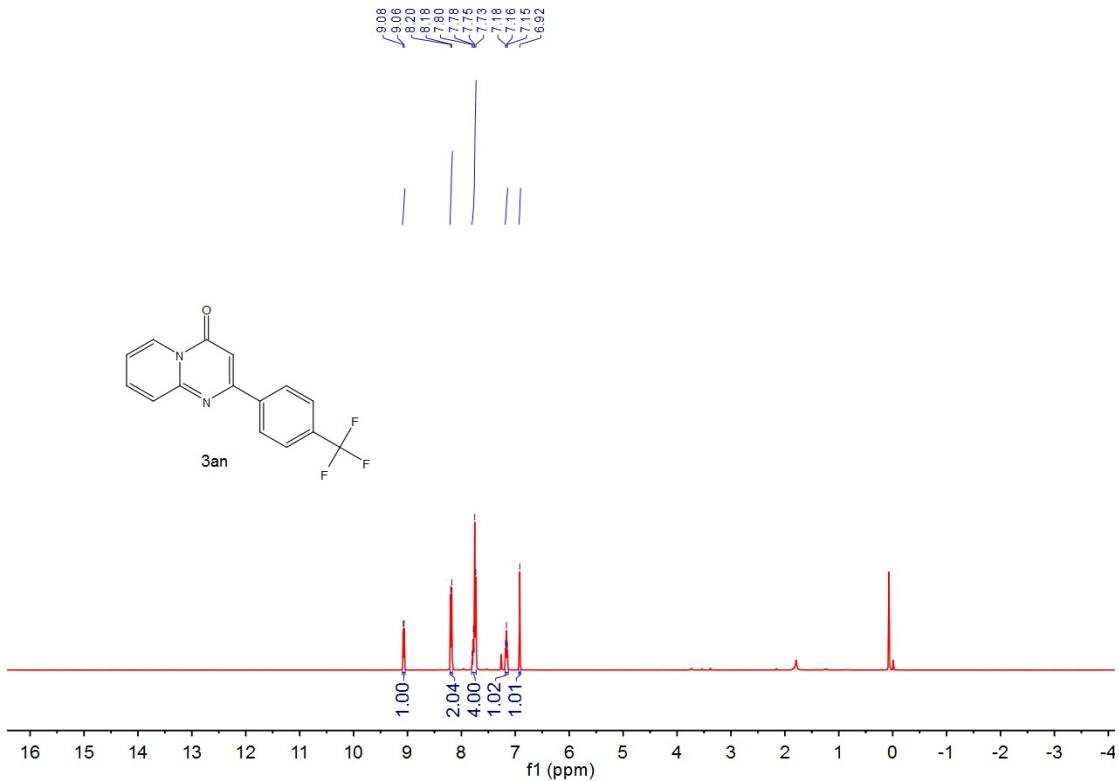


¹³C spectrum of 3am

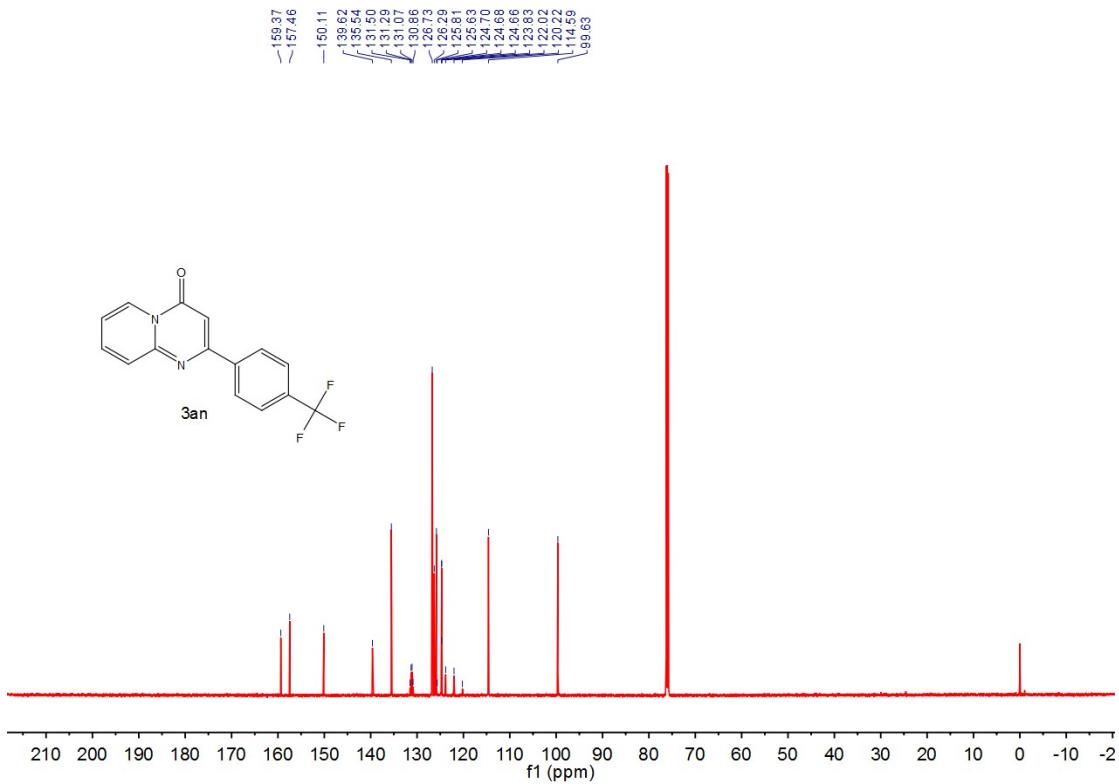


2-(4-(Trifluoromethyl)phenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3an)

¹H spectrum of 3an

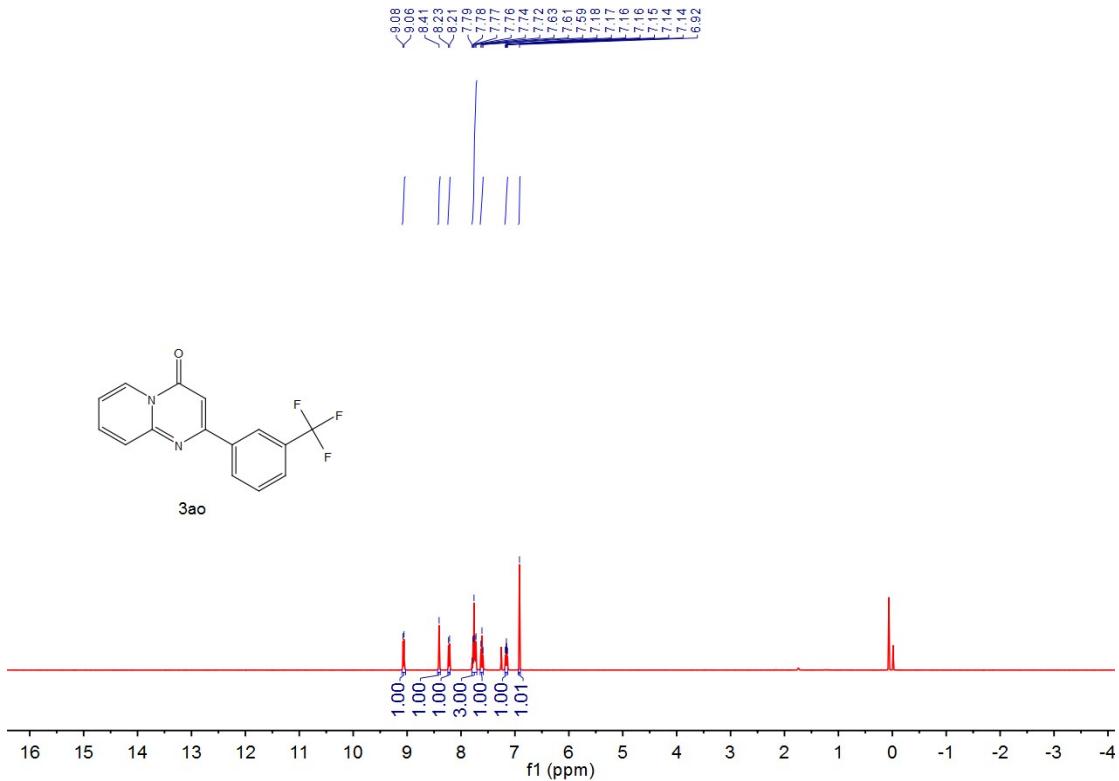


¹³C spectrum of **3an**

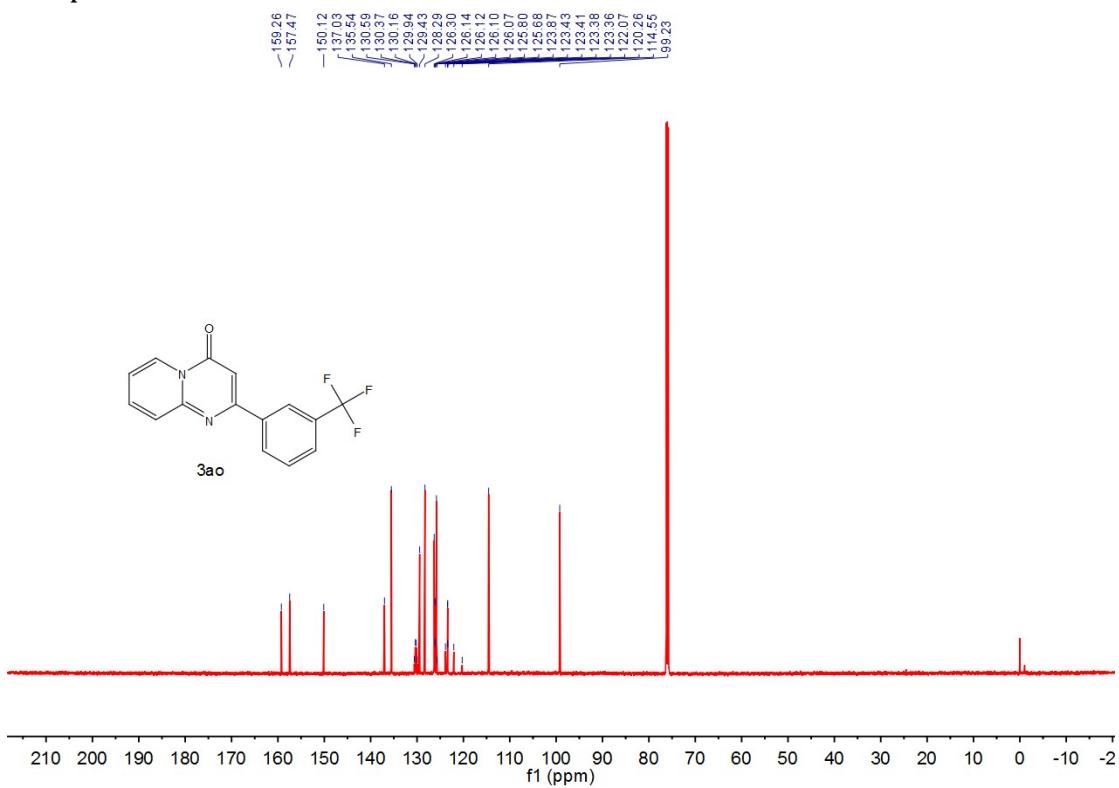


2-(3-(Trifluoromethyl)phenyl)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(3ao)

¹H spectrum of **3ao**

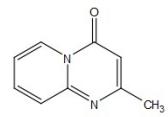
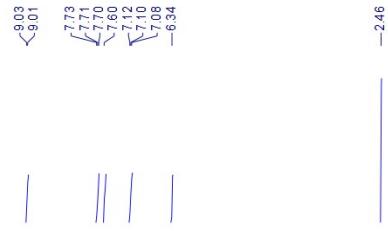


¹³C spectrum of 3ao

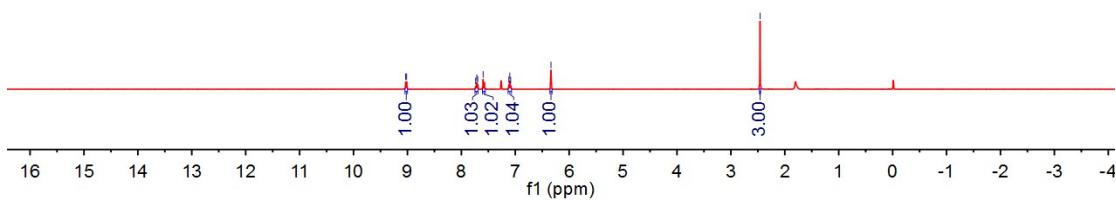


2-Methyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(3ap)

¹H spectrum of 3ap

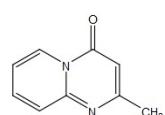


3ap

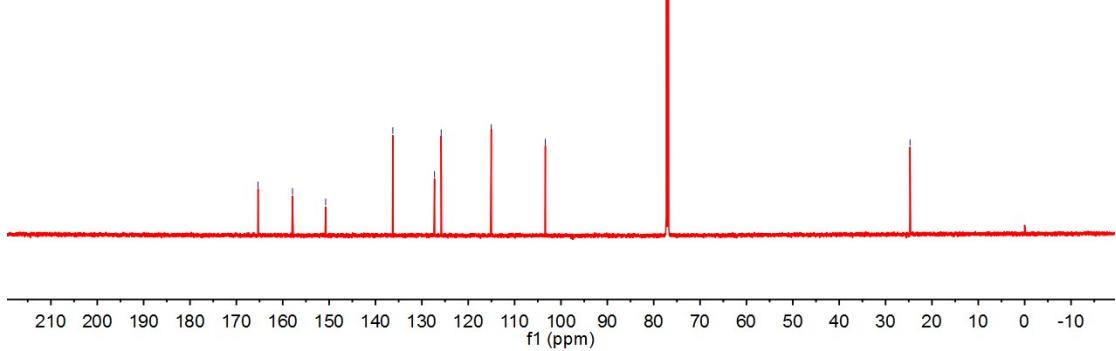


¹³C spectrum of 3ap

—165.32 —157.89 —156.74 —136.26 —127.27 ~125.84 —115.03 —103.37 —24.72

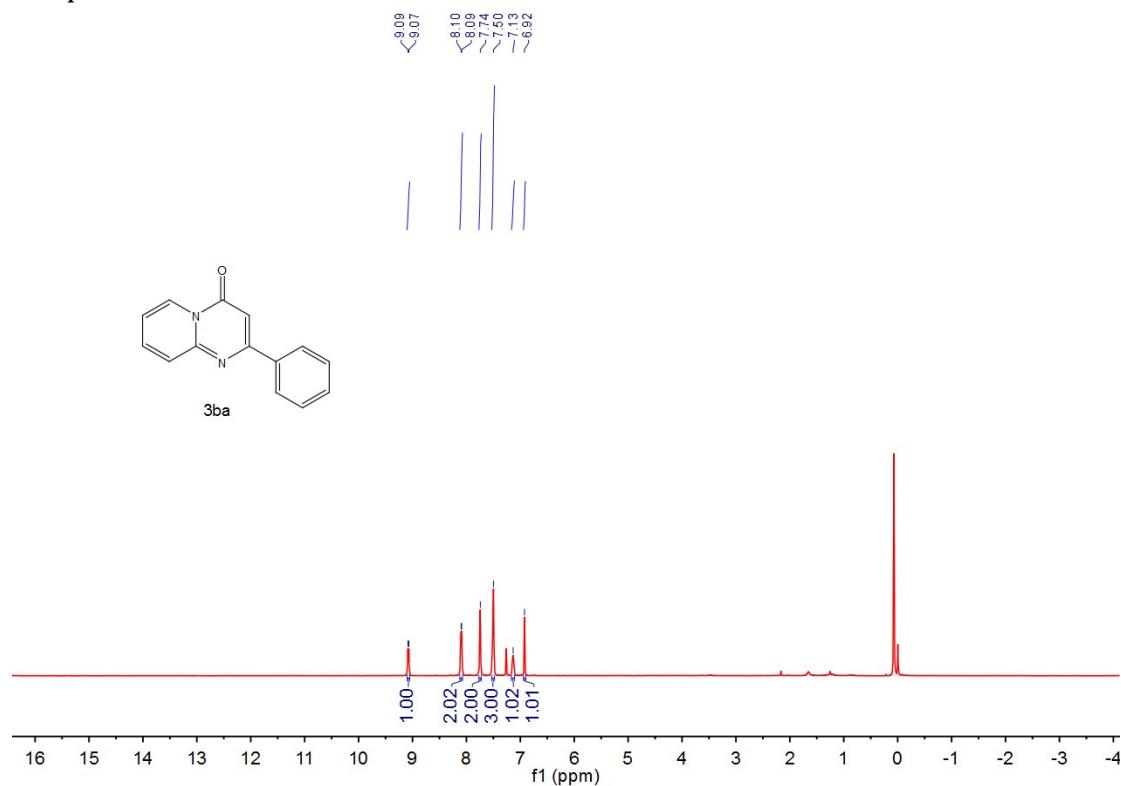


3ap

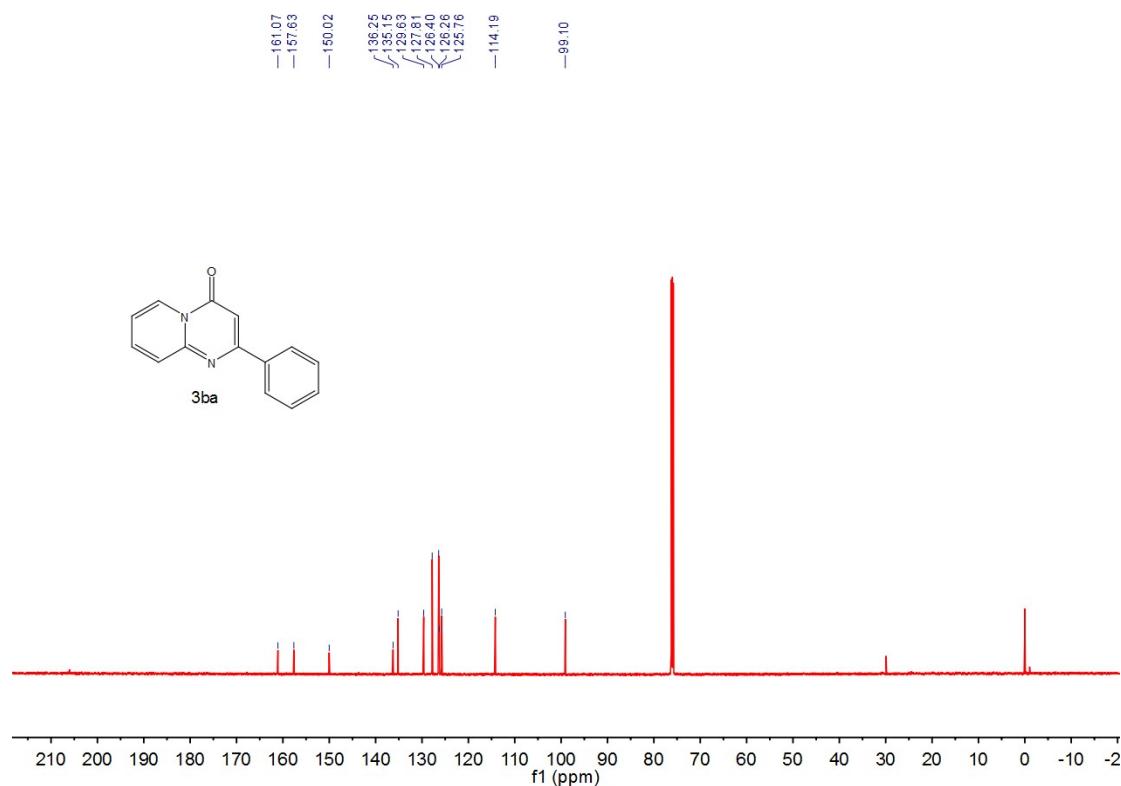


2-Phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(3ba)

¹H spectrum of **3ba**

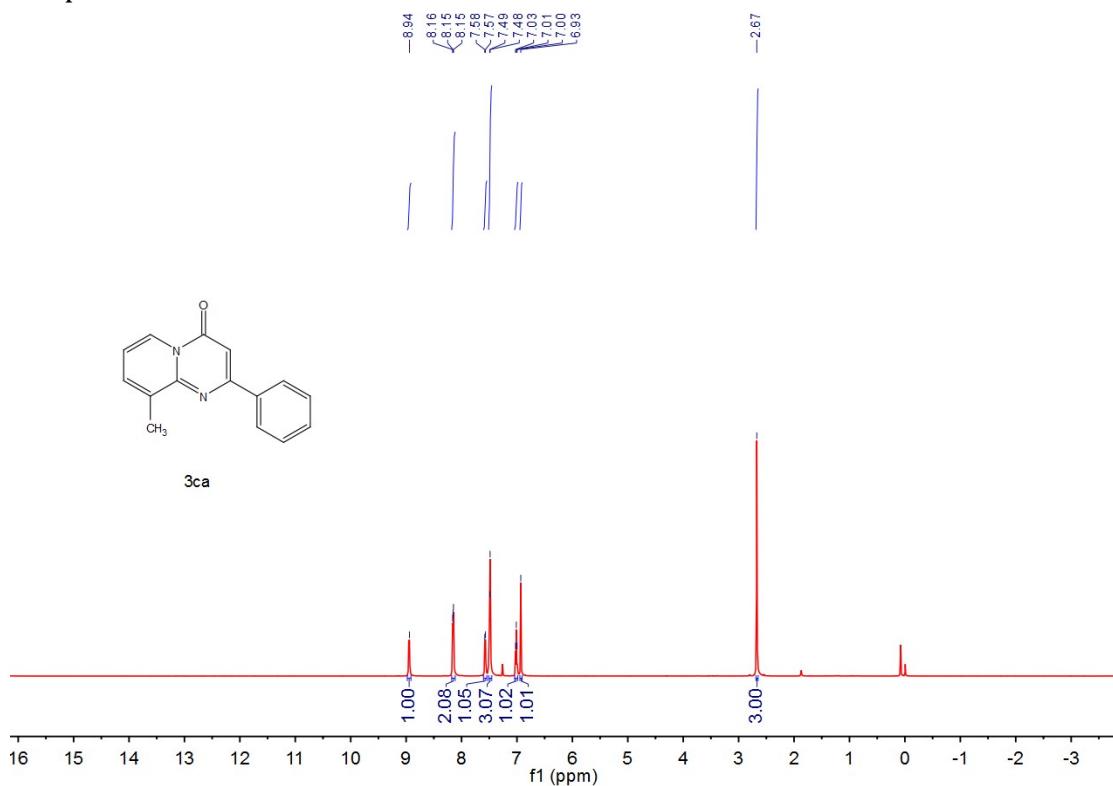


¹³C spectrum of **3ba**

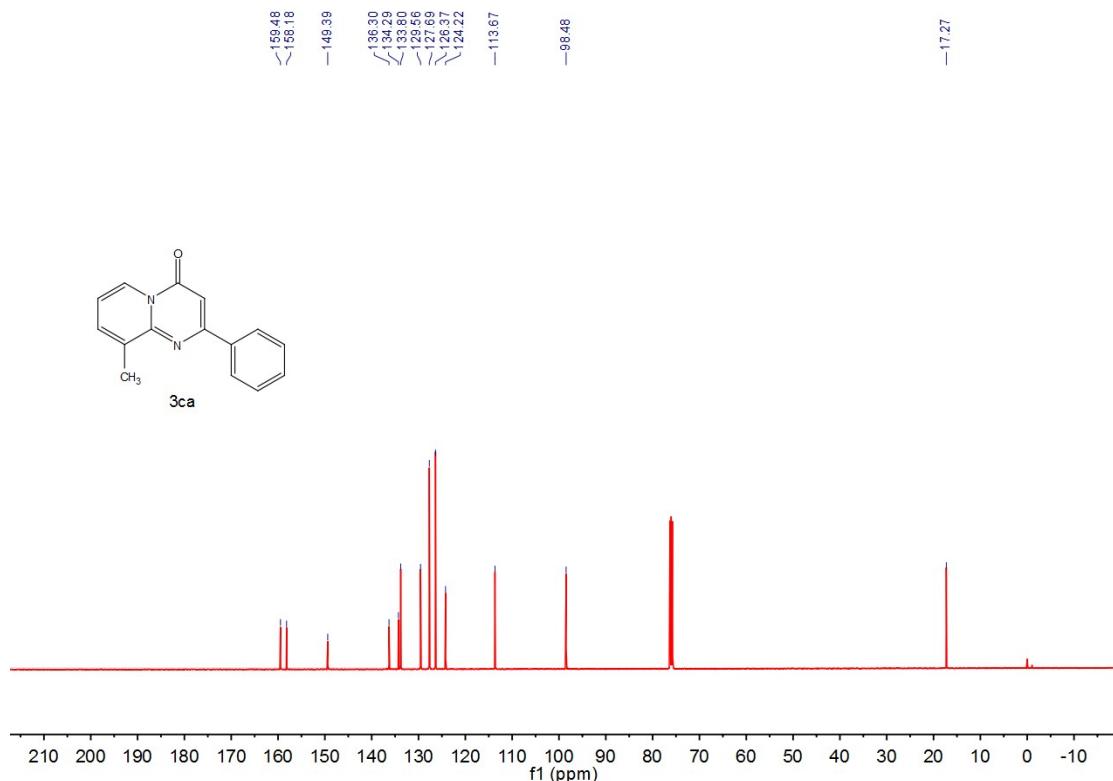


*9-Methyl-2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(3ca)*

¹H spectrum of **3ca**

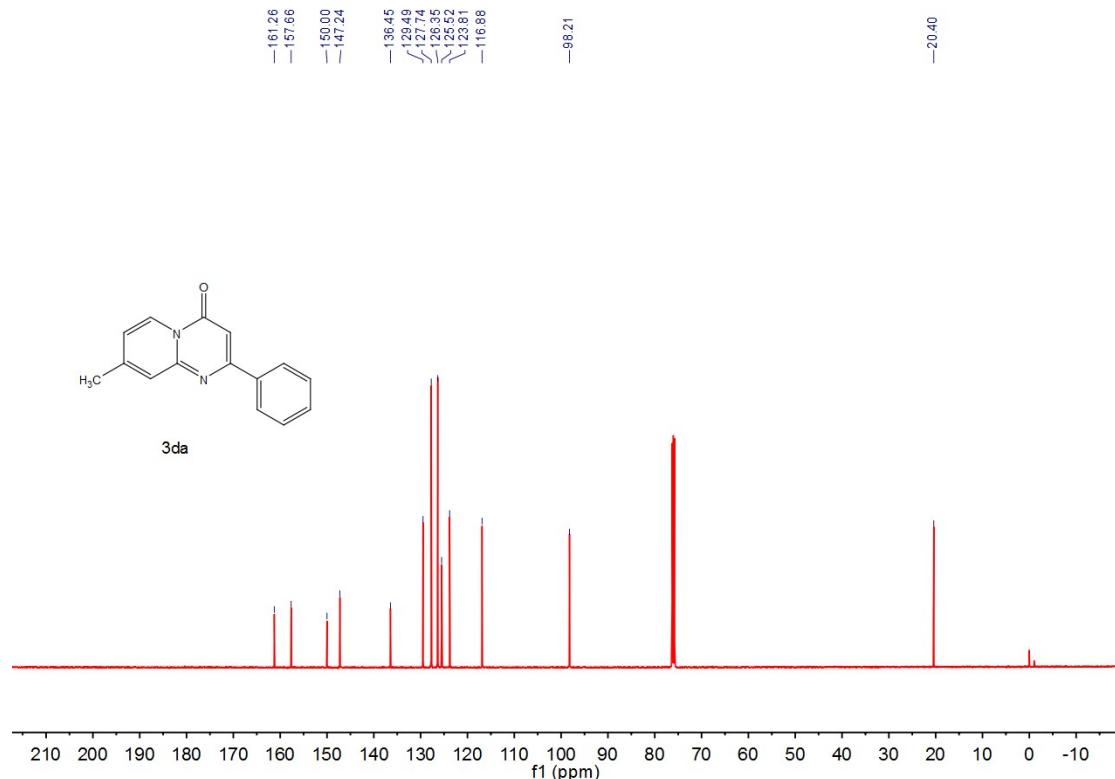
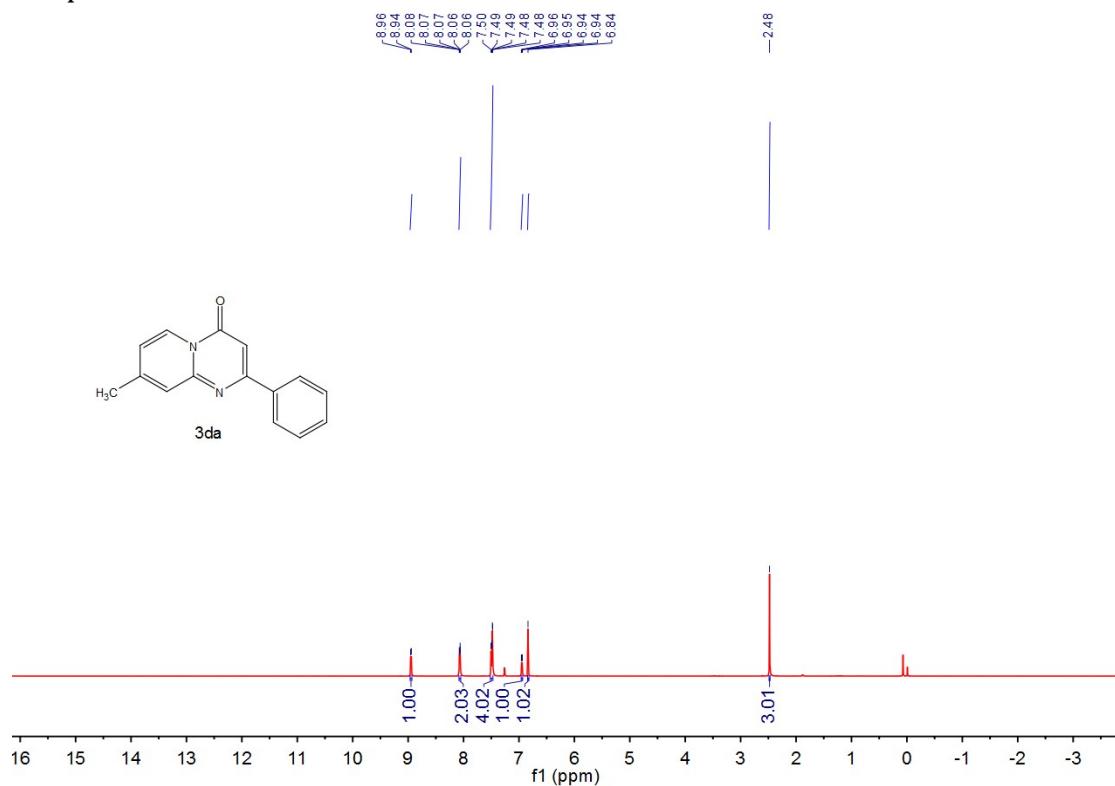


¹³C spectrum of **3ca**



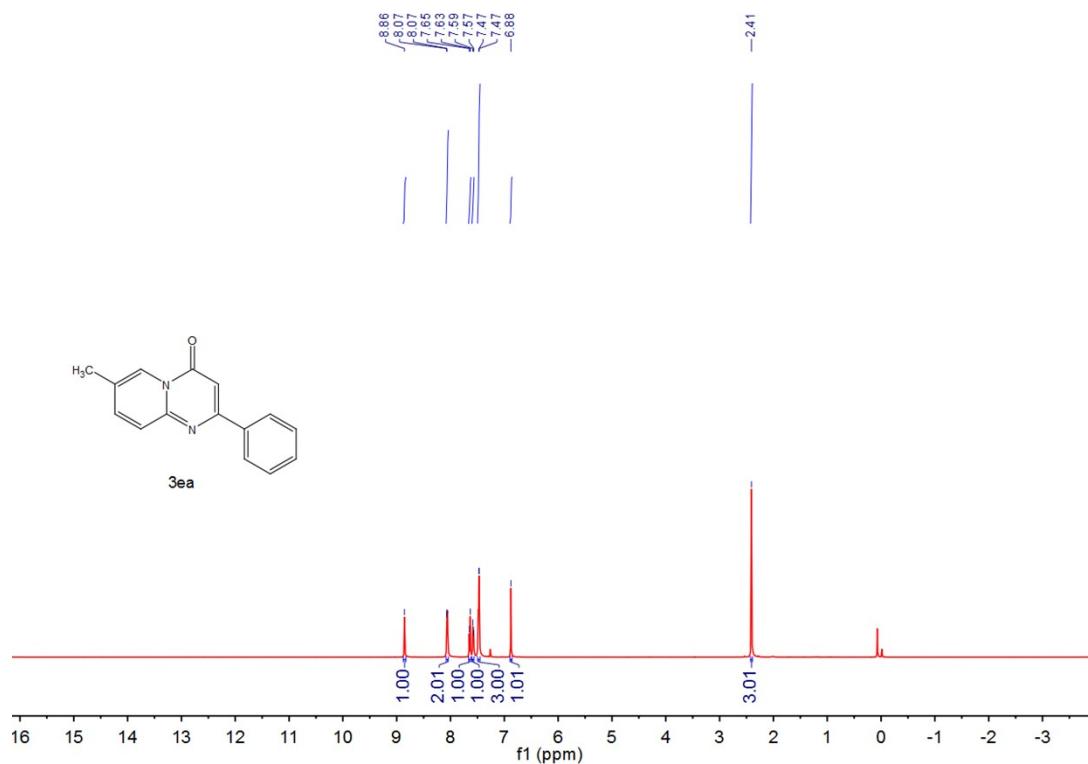
8-Methyl-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one (3da)

¹H spectrum of **3da**

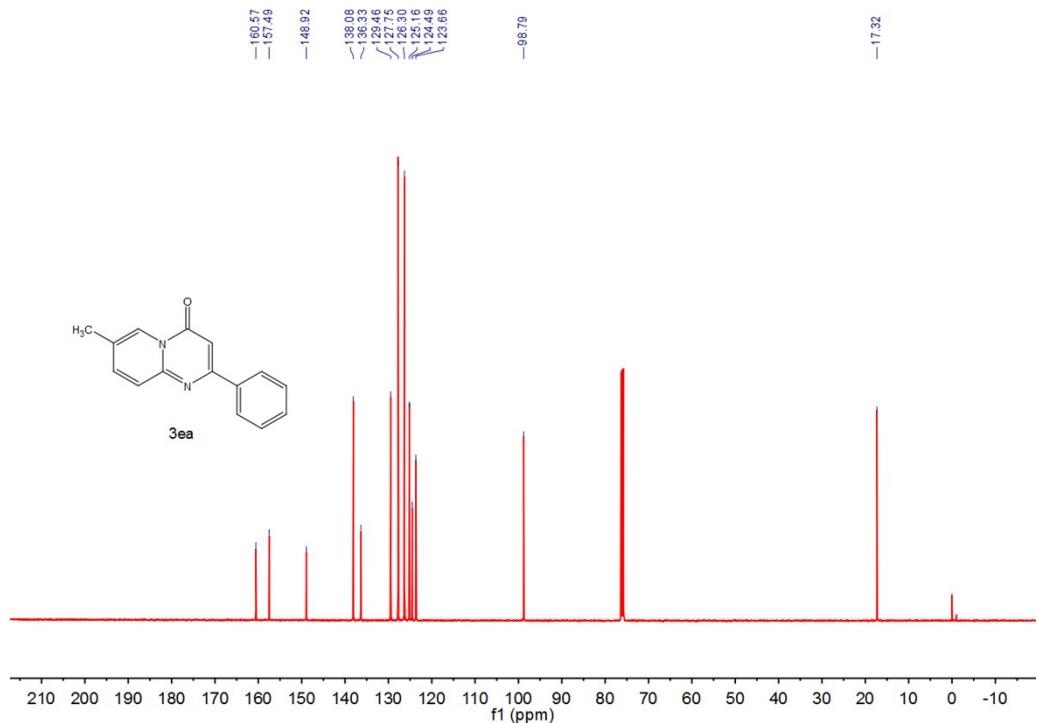


7-Methyl-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(3ea)

¹H spectrum of 3ea

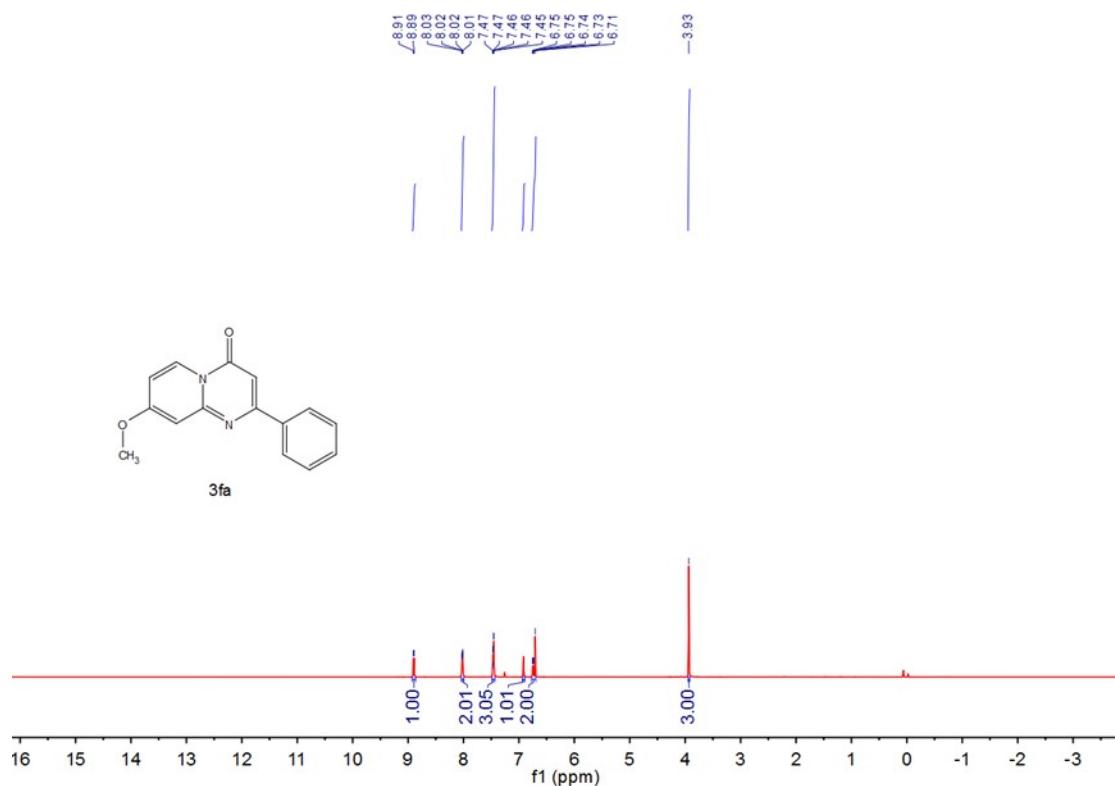


¹³C spectrum of 3ea

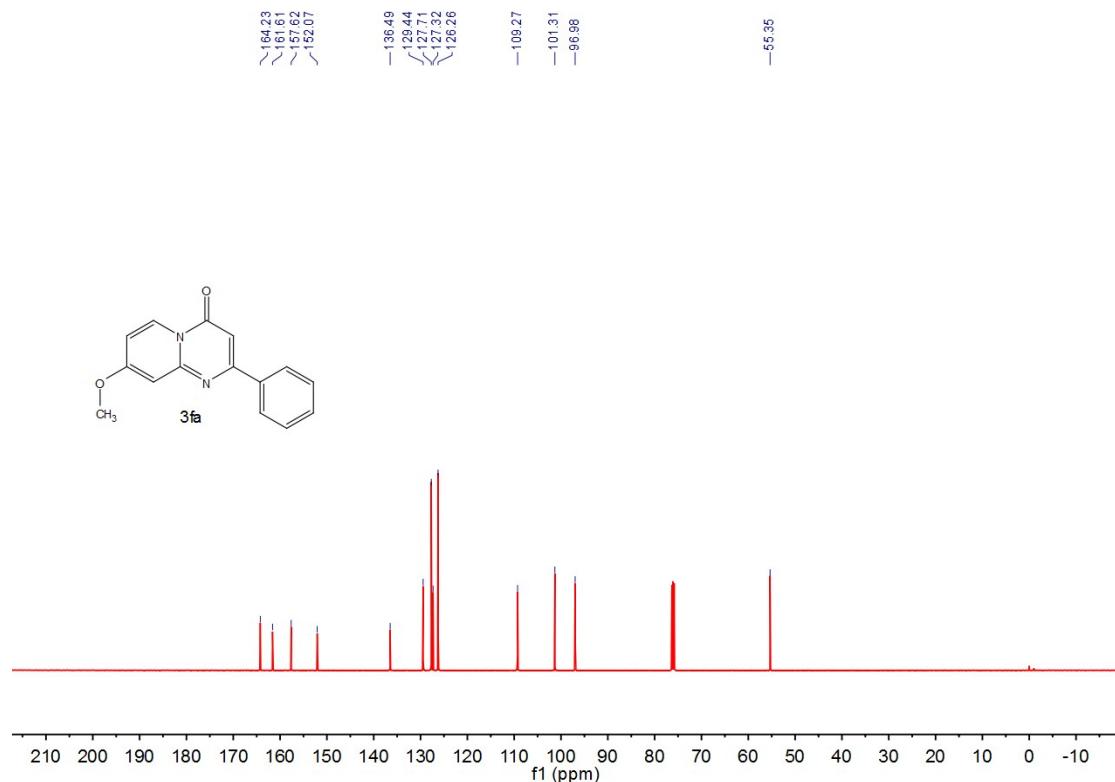


8-Methoxy-2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-one(3fa)

¹H spectrum of **3fa**

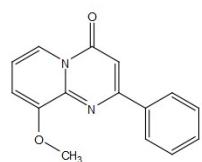


¹³C spectrum of **3fa**

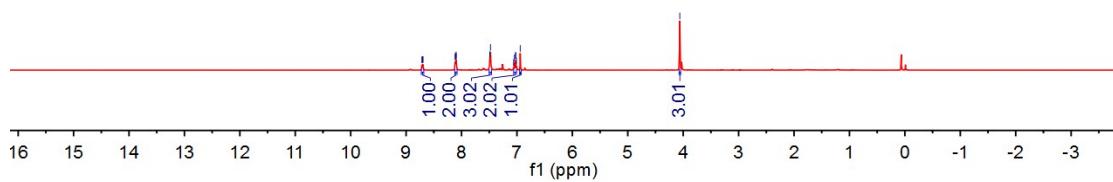


9-Methoxy-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(3ga)

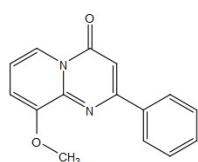
¹H spectrum of 3ga



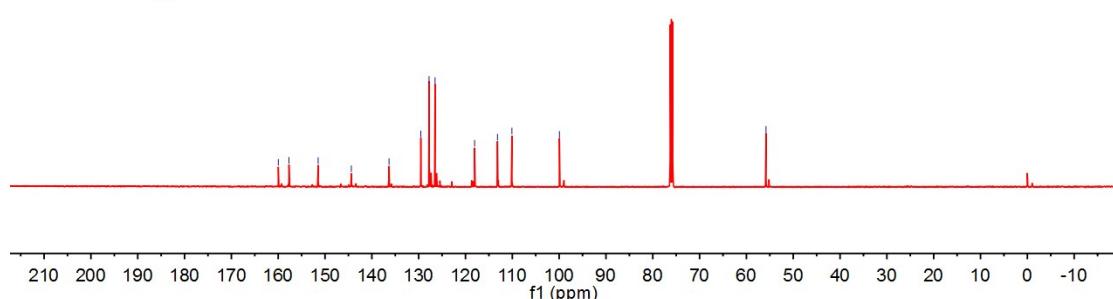
3qa



¹³C spectrum of 3ga

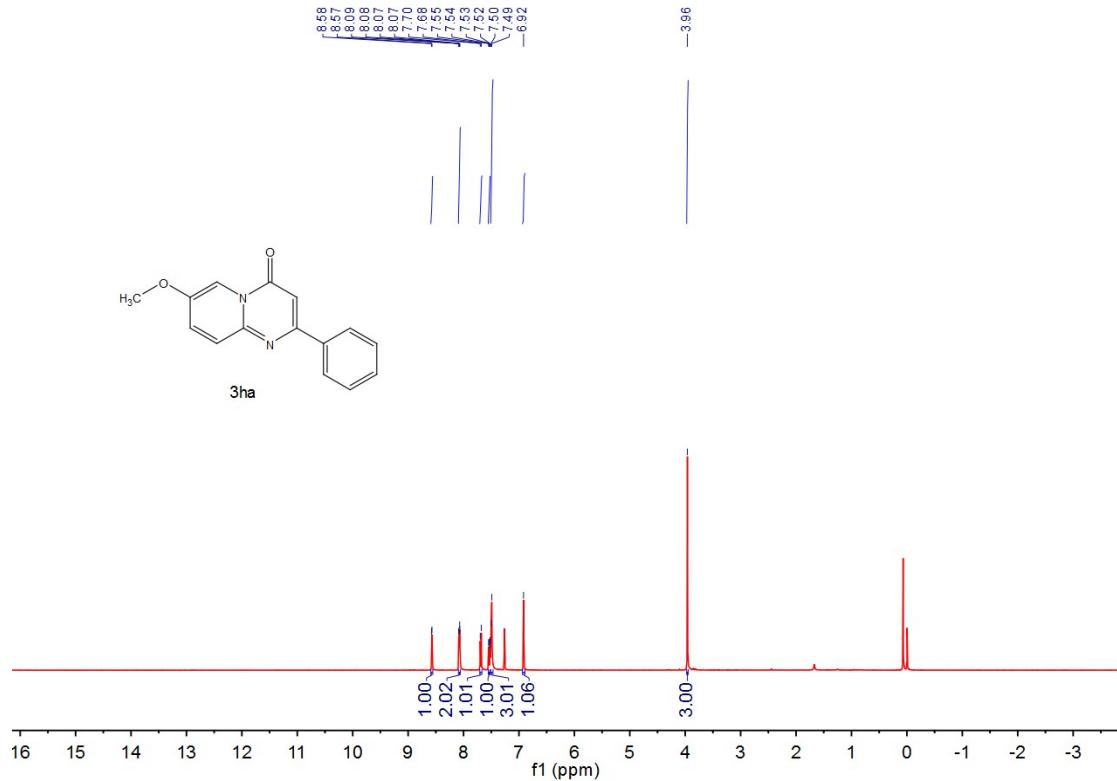


3ga

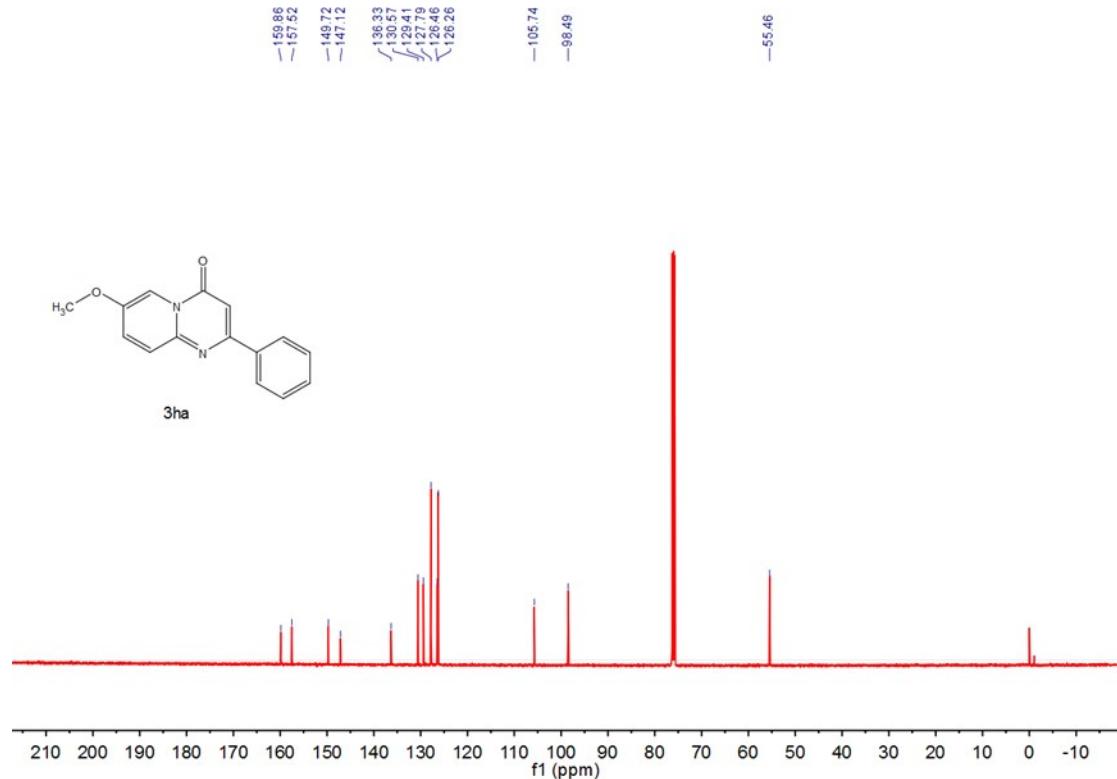


7-Methoxy-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(3ha)

¹H spectrum of 3ha

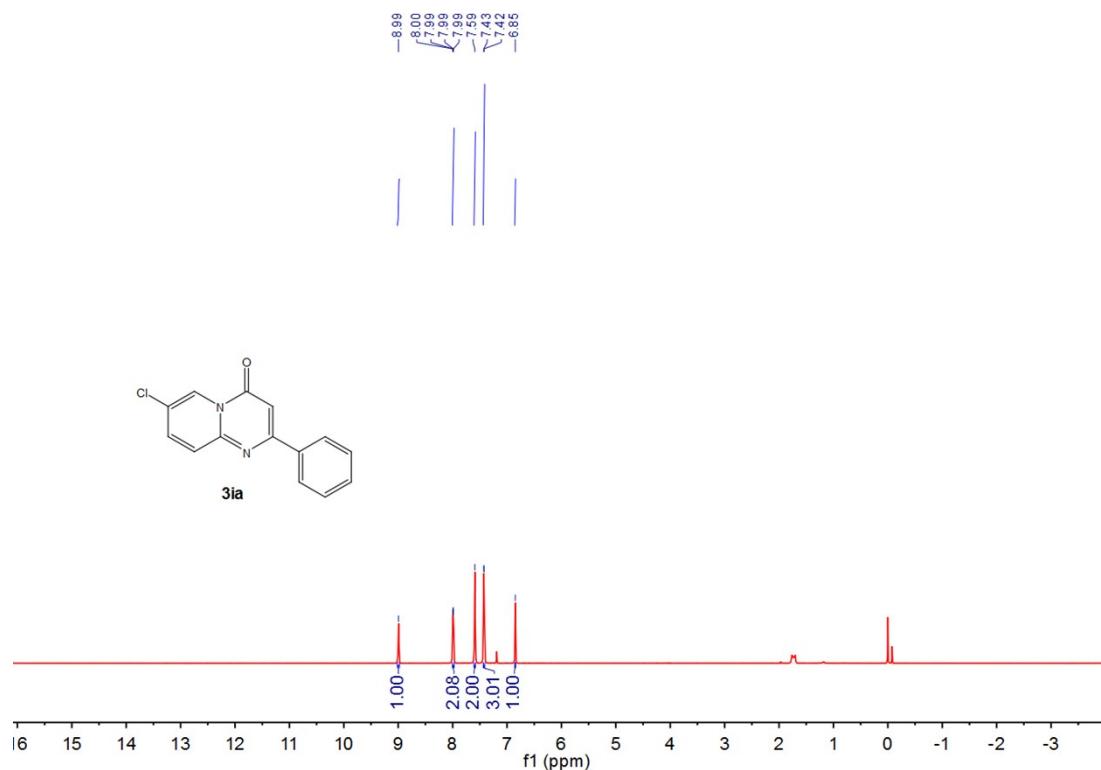


¹³C spectrum of **3ha**

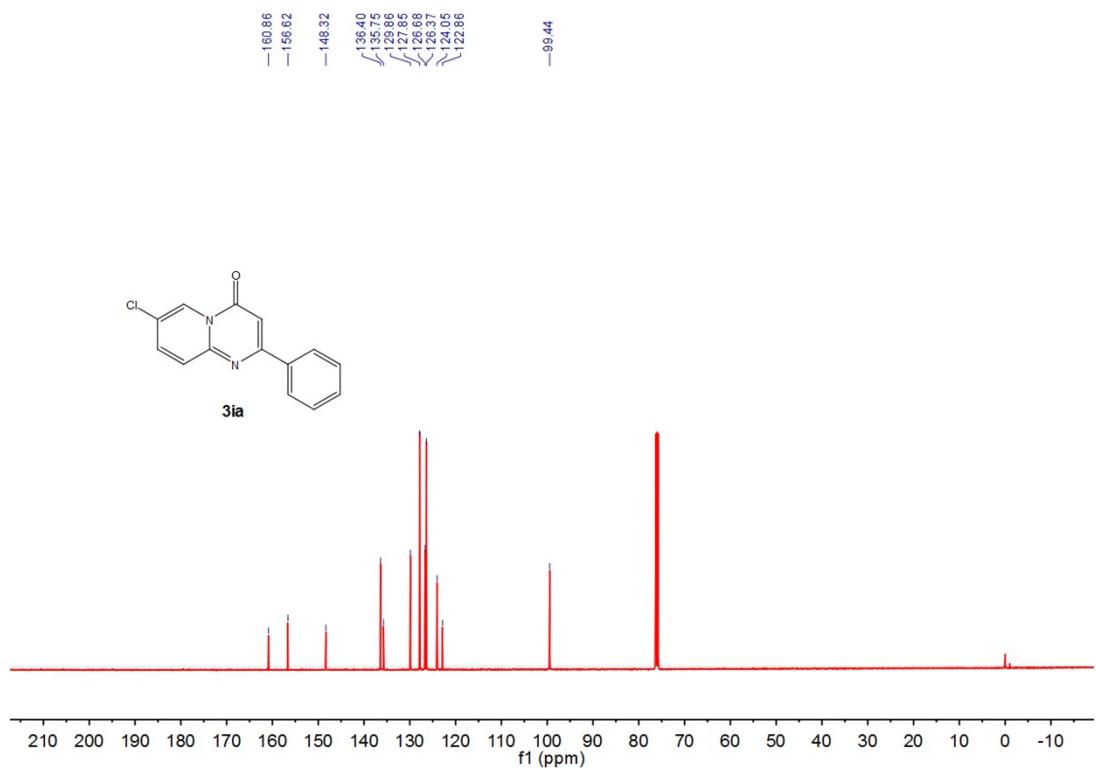


7-Chloro-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(**3ia**)

¹H spectrum of **3ia**

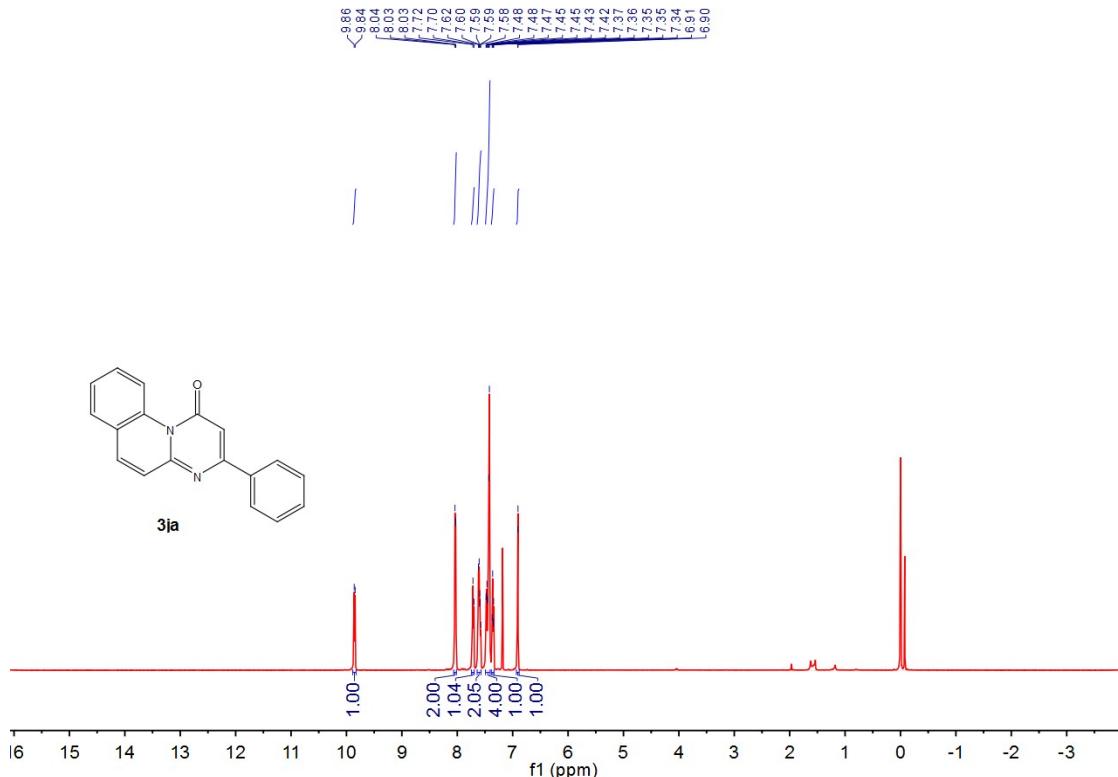


^{13}C spectrum of **3ia**

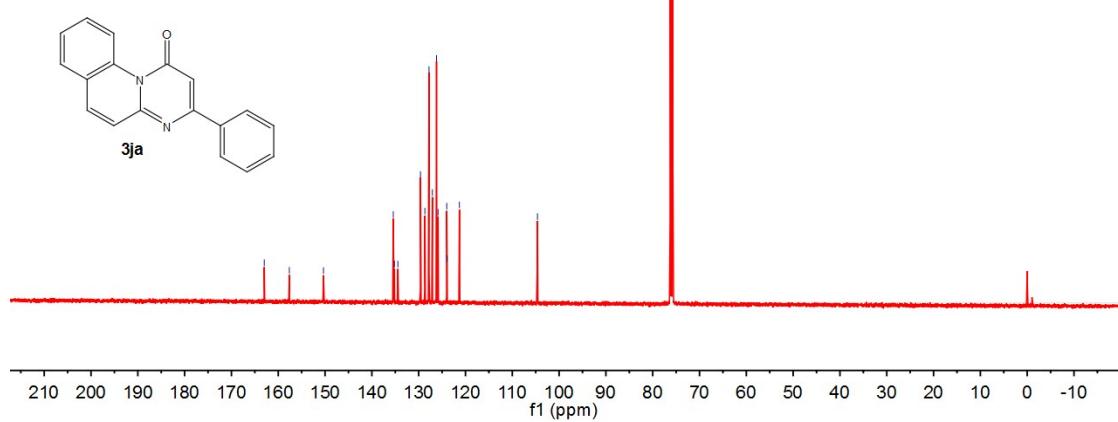


*3-Phenyl-1*H*-pyrimido[1,2-*a*]quinolin-1-one(3ja)*

^1H spectrum of **3ja**

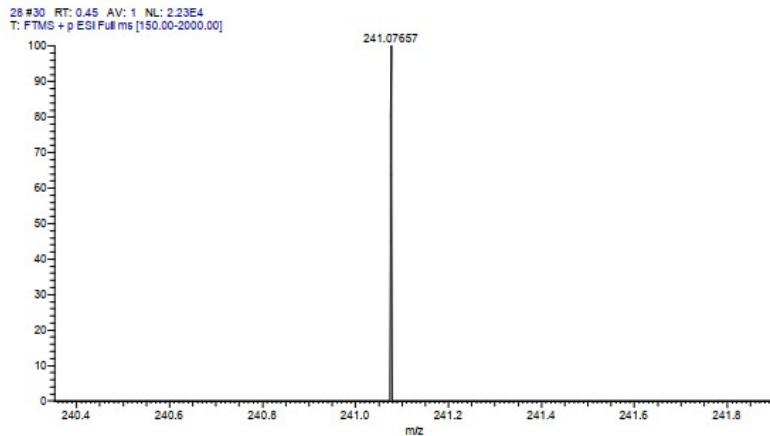


¹³C spectrum of 3ja

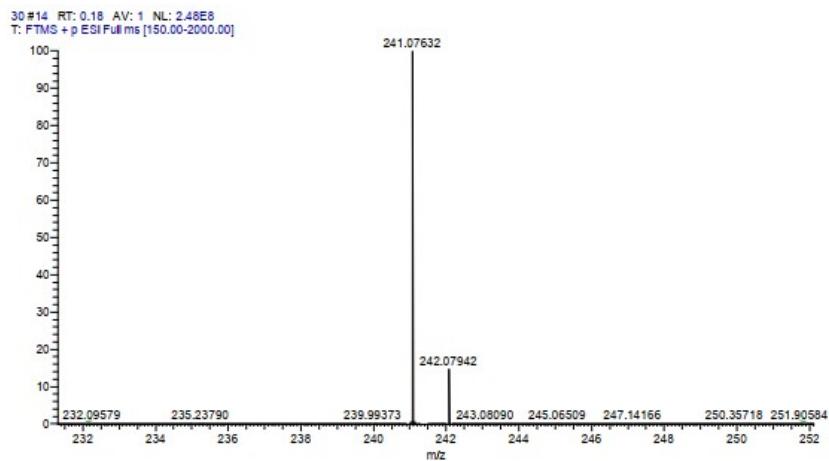


2. High-resolution mass spectra of new compounds

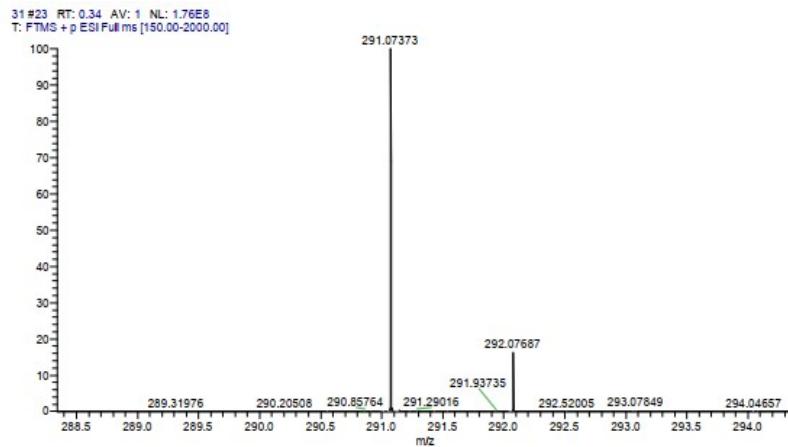
2-(3-Fluorophenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3ak)



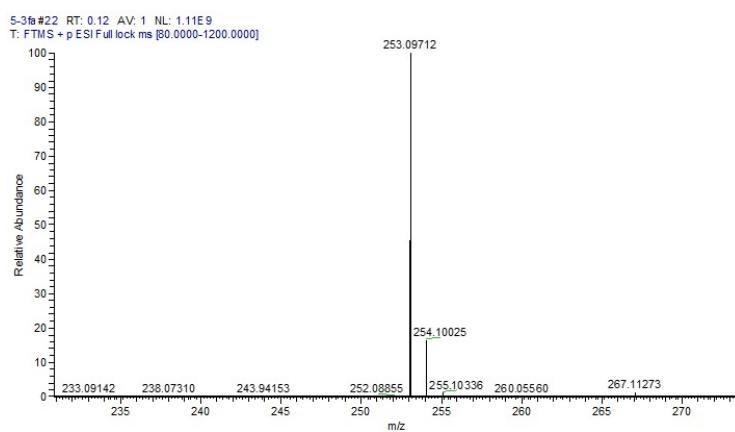
2-(2-Fluorophenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3al)



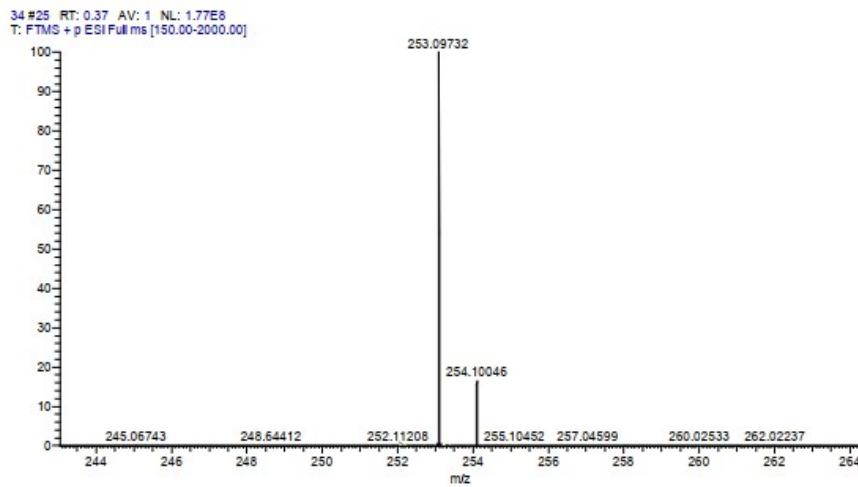
2-(3-(Trifluoromethyl)phenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3ao)



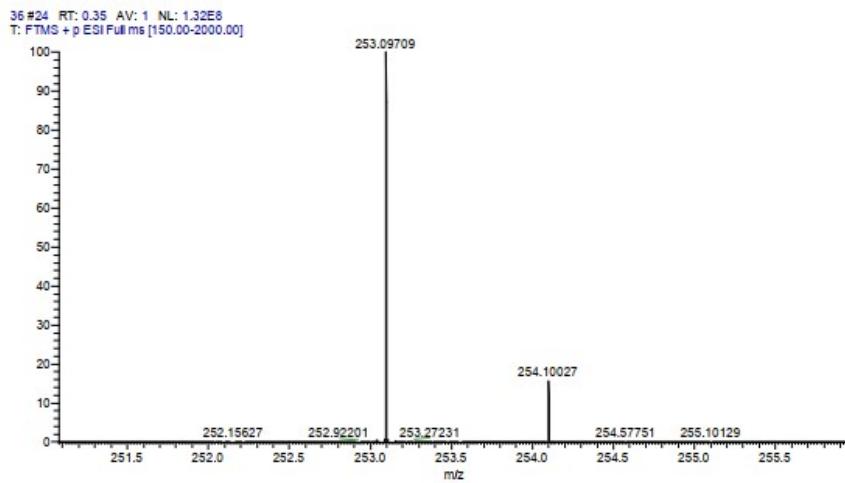
8-Methoxy-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(3fa)



9-Methoxy-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(3ga)

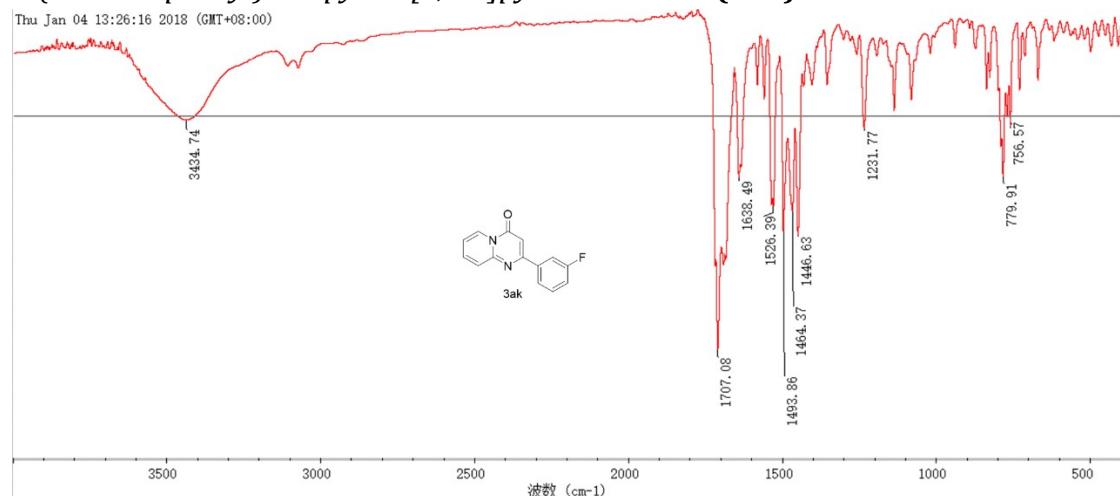


7-Methoxy-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(3ha)

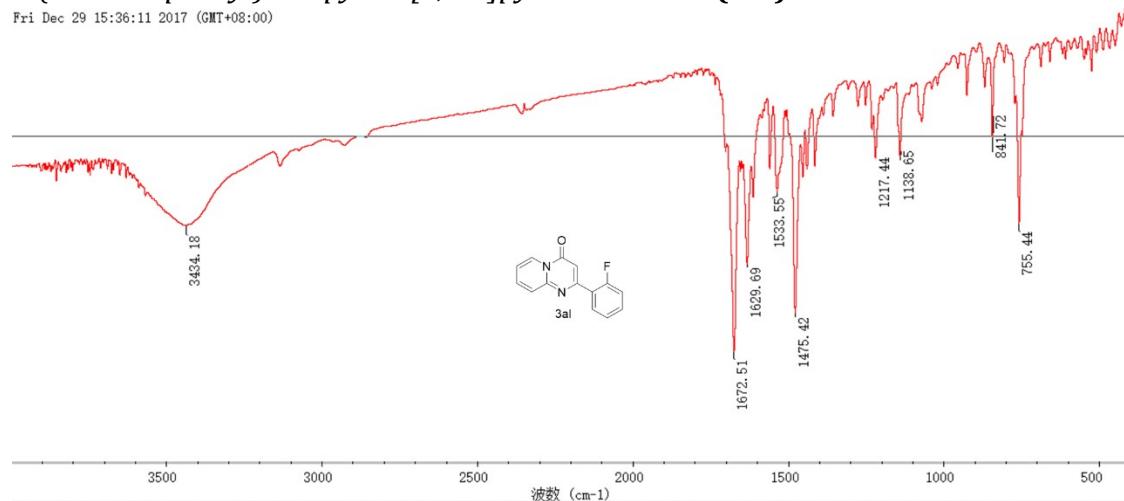


3. IR spectra of new compounds

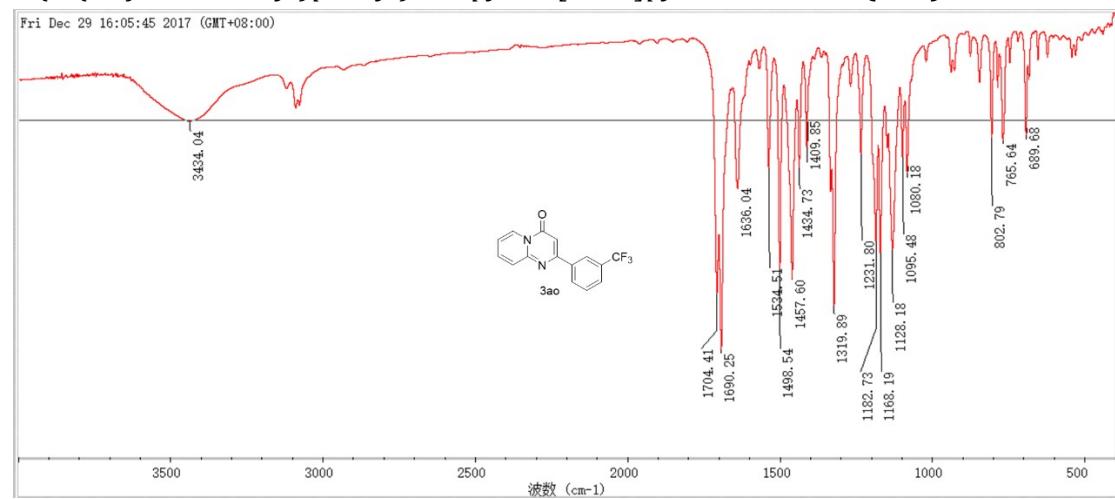
2-(3-Fluorophenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3ak)



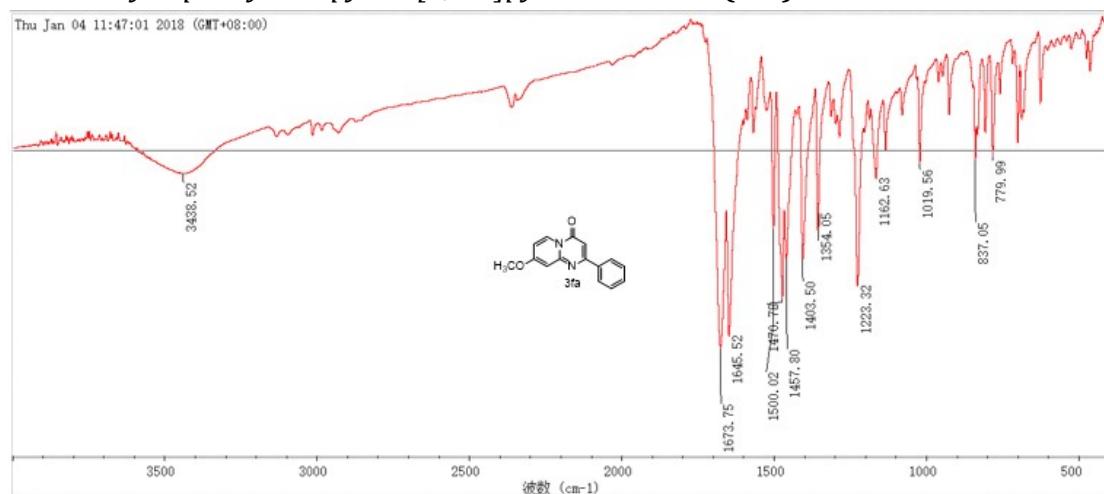
2-(2-Fluorophenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3al)



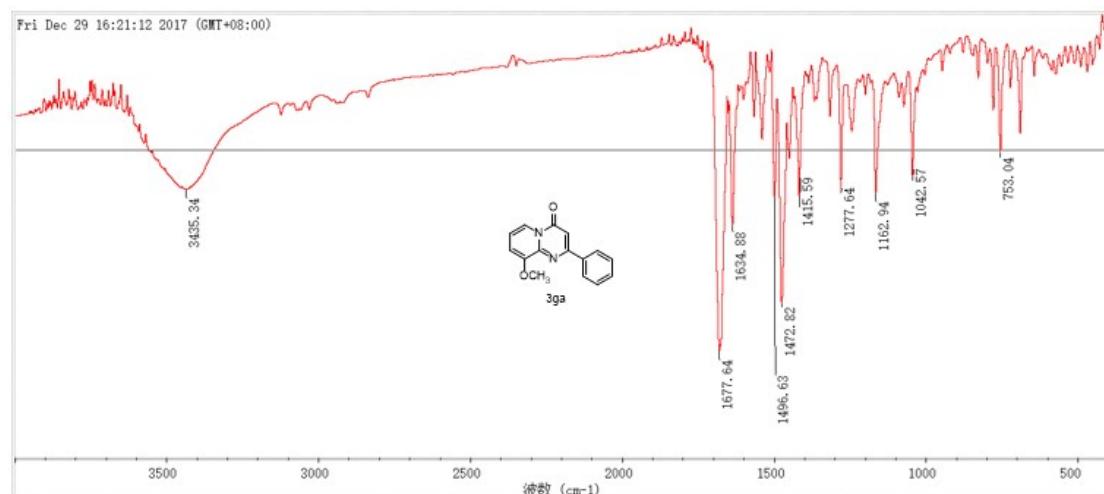
2-(3-(Trifluoromethyl)phenyl)-4H-pyrido[1,2-a]pyrimidin-4-one(3ao)



8-Methoxy-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(3fa)



9-Methoxy-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(3ga)



7-Methoxy-2-phenyl-4H-pyrido[1,2-a]pyrimidin-4-one(3ha)

