

# Supplementary Information

**Fast, solvent-free, and highly efficient synthesis of pyrazolo[3,4-*b*]pyridines using microwave irradiation and KHSO<sub>4</sub> as a reusable free catalyst**

Jinjing Qin, Zhenhua Li\*, Xiaomeng Sun, Yi Jin and Weike Su

College of Pharmaceutical Sciences, Zhejiang University of Technology, 310014 Hangzhou, PR China; E-Mail: lizhenhua@zjut.edu.cn

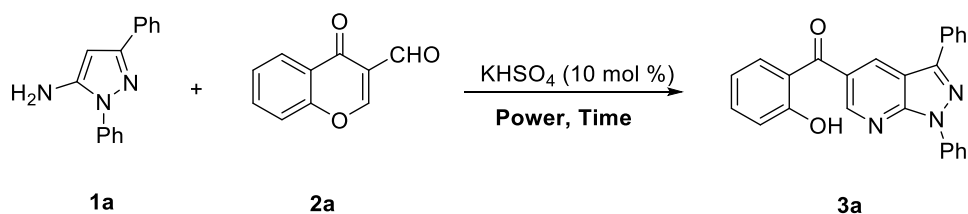
**Experimental section, <sup>1</sup>H and <sup>13</sup>C NMR spectra of prepared compounds**

## **Table of contents**

- 1. Optimization of reaction conditions**
- 2. Copies of <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra**

## 1. Optimization of reaction conditions

**Table S1:** The influences of the microwave irradiation power and reaction time<sup>a</sup>

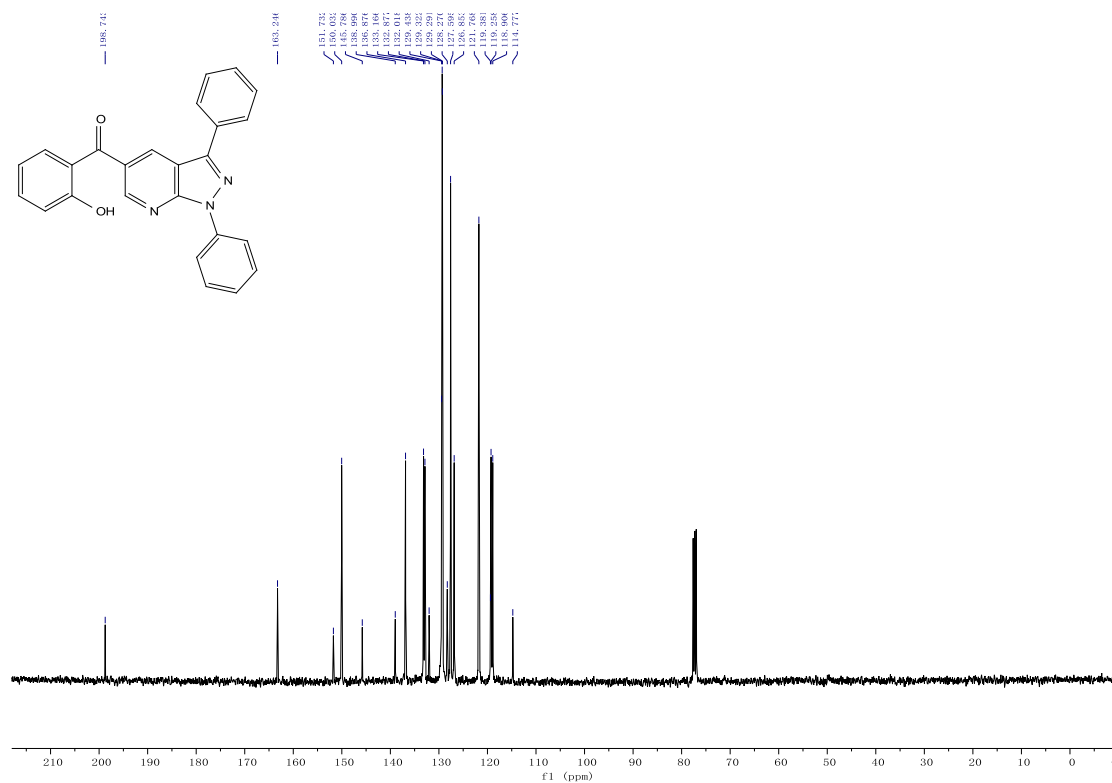
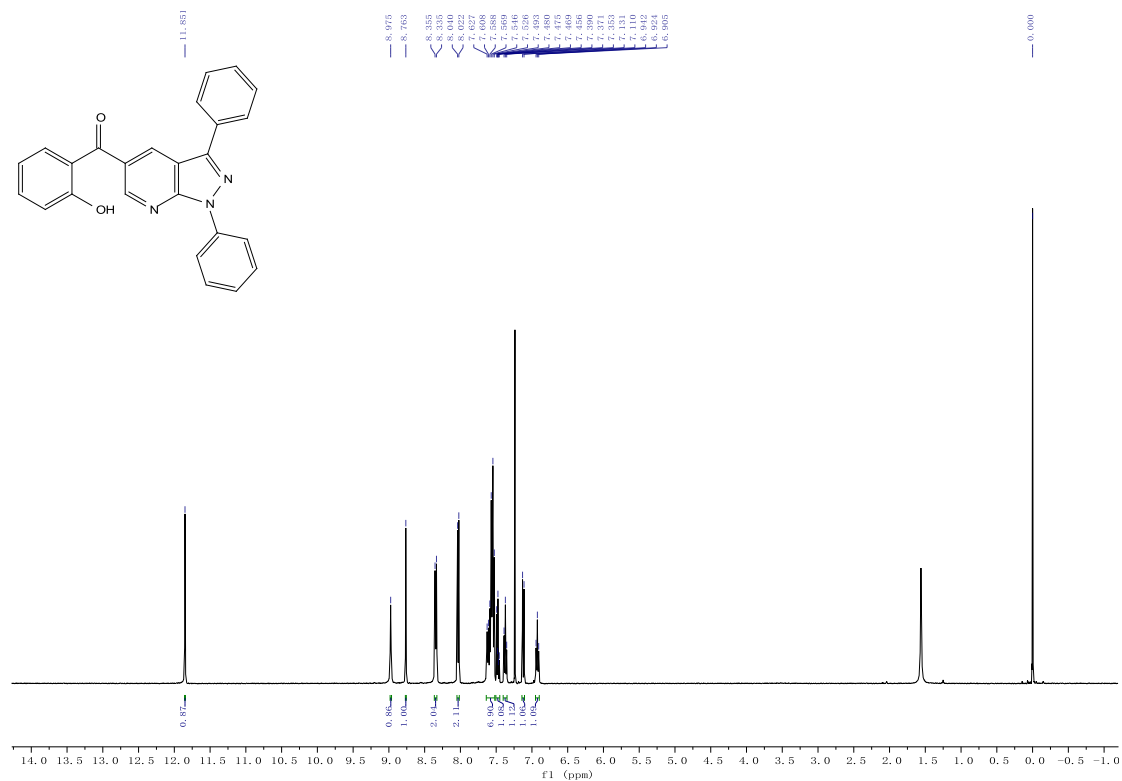


Entry	Microwave power (W)	Reaction time (min)	Yield <sup>b</sup> (%)
1	550	10	85
2	400	10	Trace
3	400	20	10
4	400	30	30
5	400	60	50
6	550	5	60
7	550	20	95
8	550	30	93
9	700	10	96
<b>10</b>	<b>700</b>	<b>5</b>	<b>97</b>
11	700	3	86
12	700	1	10

<sup>a</sup>The reaction standard conditions: **1a** (2 mmol), **2a** (2 mmol) and KHSO<sub>4</sub> (10 mol %) were placed in a ceramic crucible, grinded by a pestle for 2 min, reacted under microwave irradiation at specific microwave power for specific time without stir. <sup>b</sup>Isolated yields.

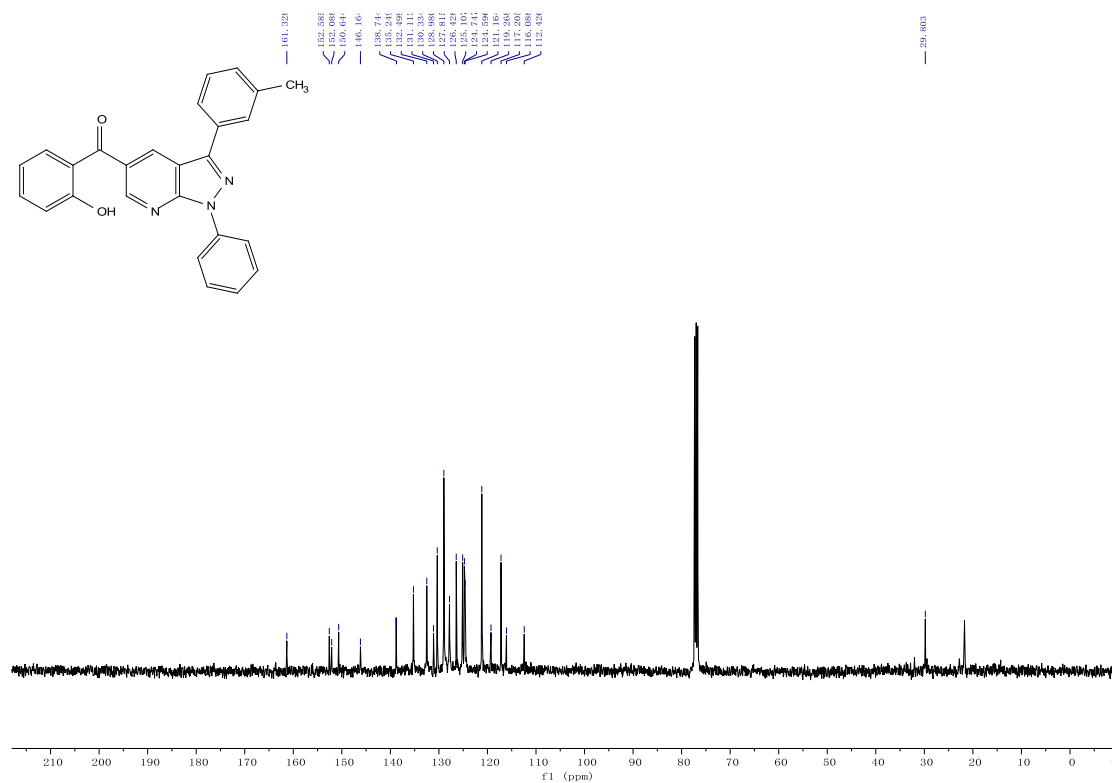
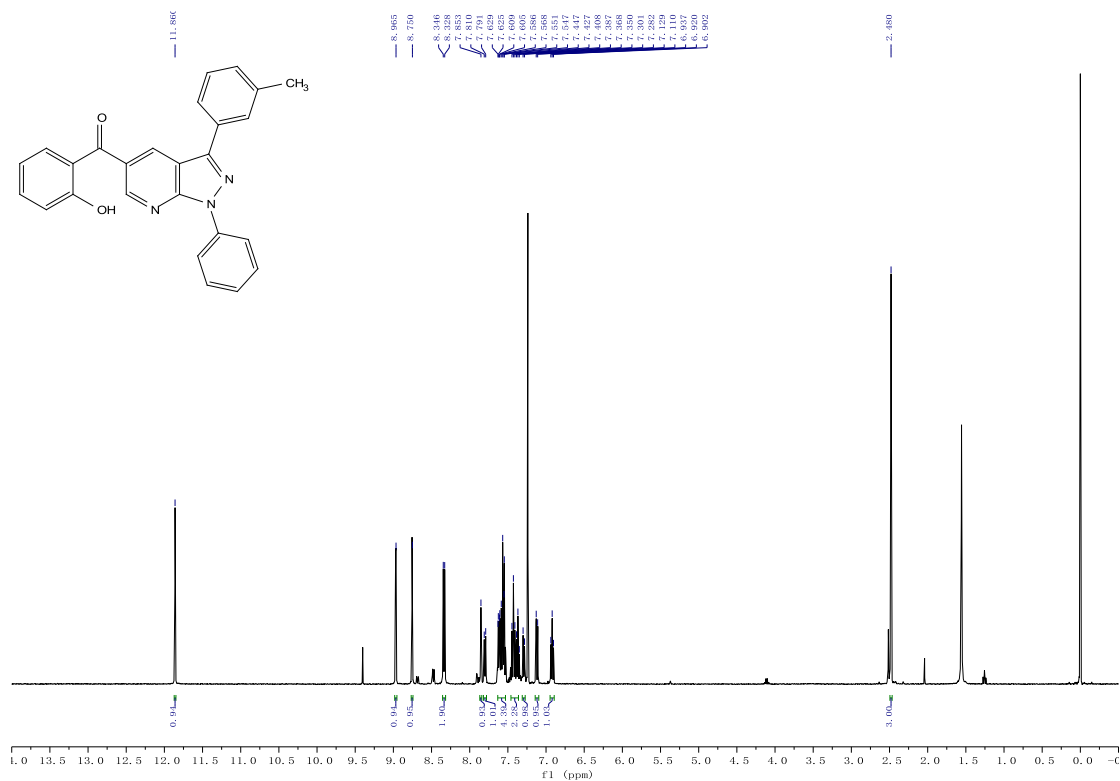
## 2. Copies of $^1\text{H}$ NMR and $^{13}\text{C}$ NMR spectra

### (1,3-diphenyl-1*H*-pyrazolo[3,4-*b*]pyridin-5-yl)(2-hydroxyphenyl)methanone (3a).

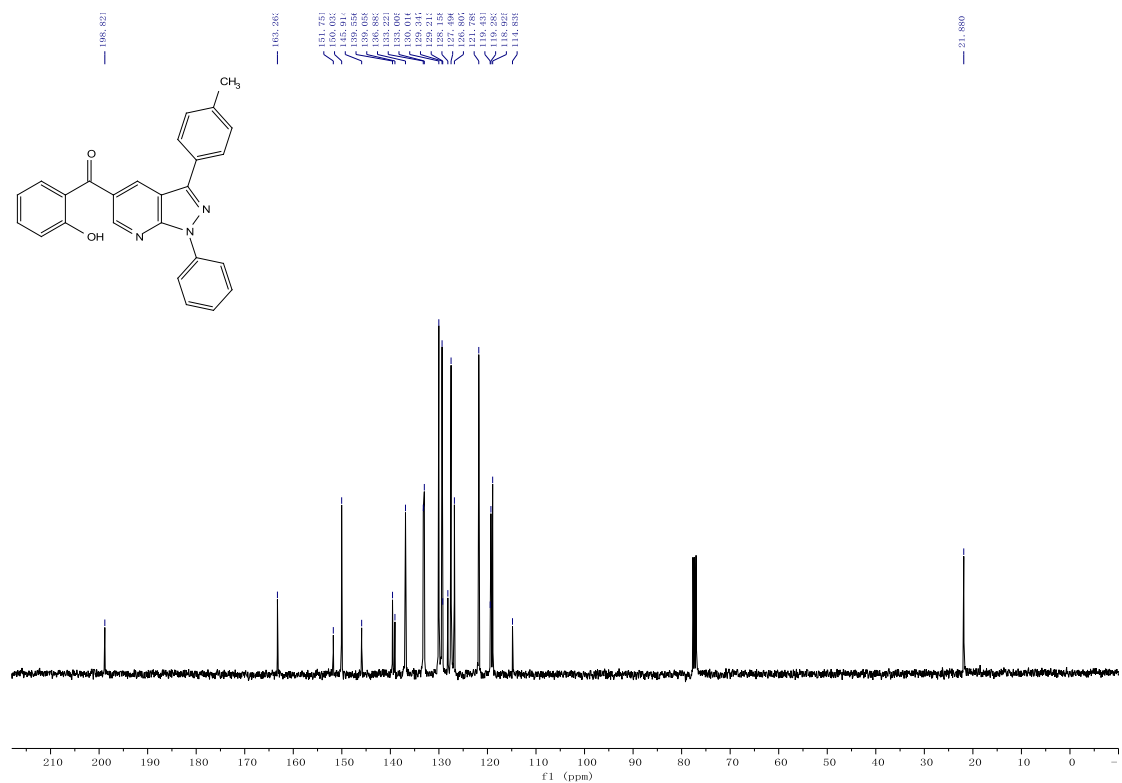
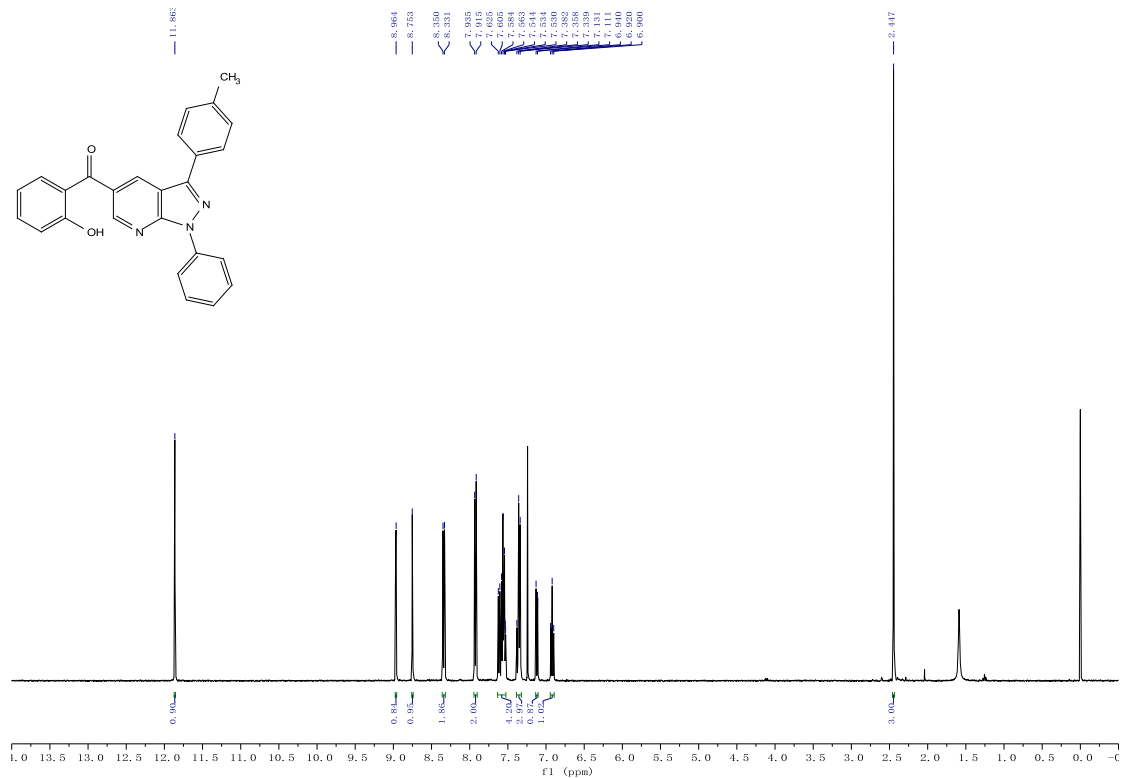


(2-hydroxyphenyl)(1-phenyl-3-(*m*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridin-5-yl)methanone

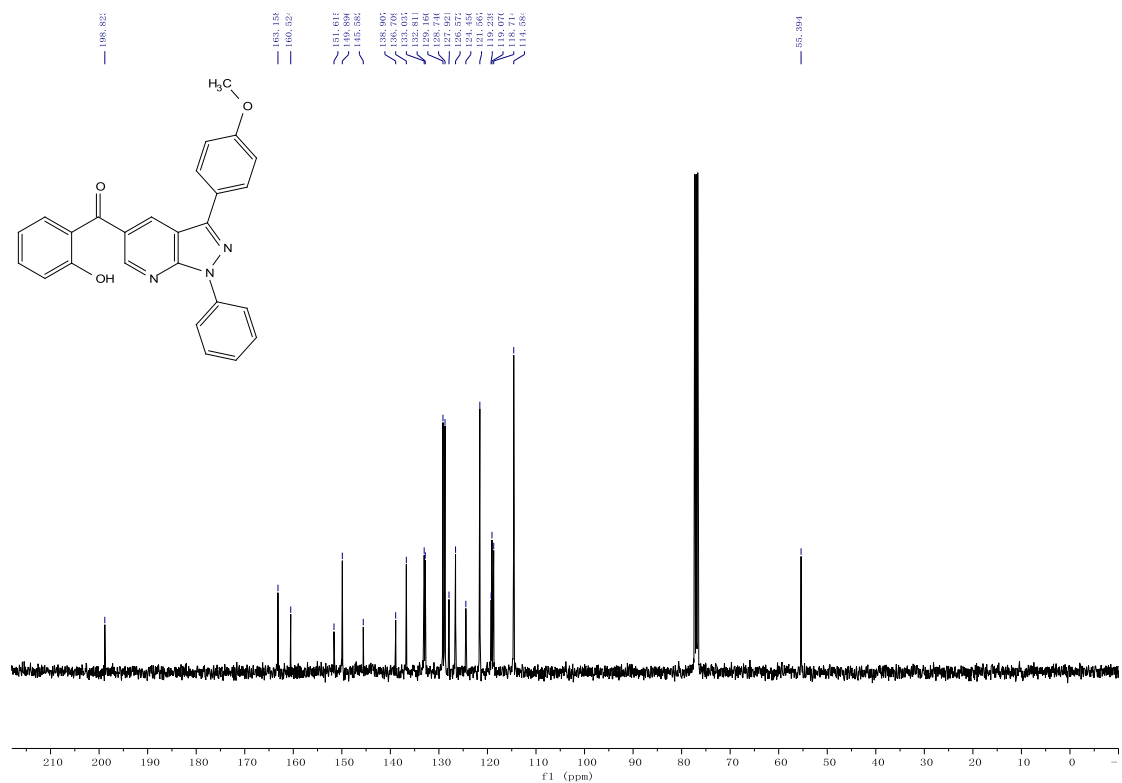
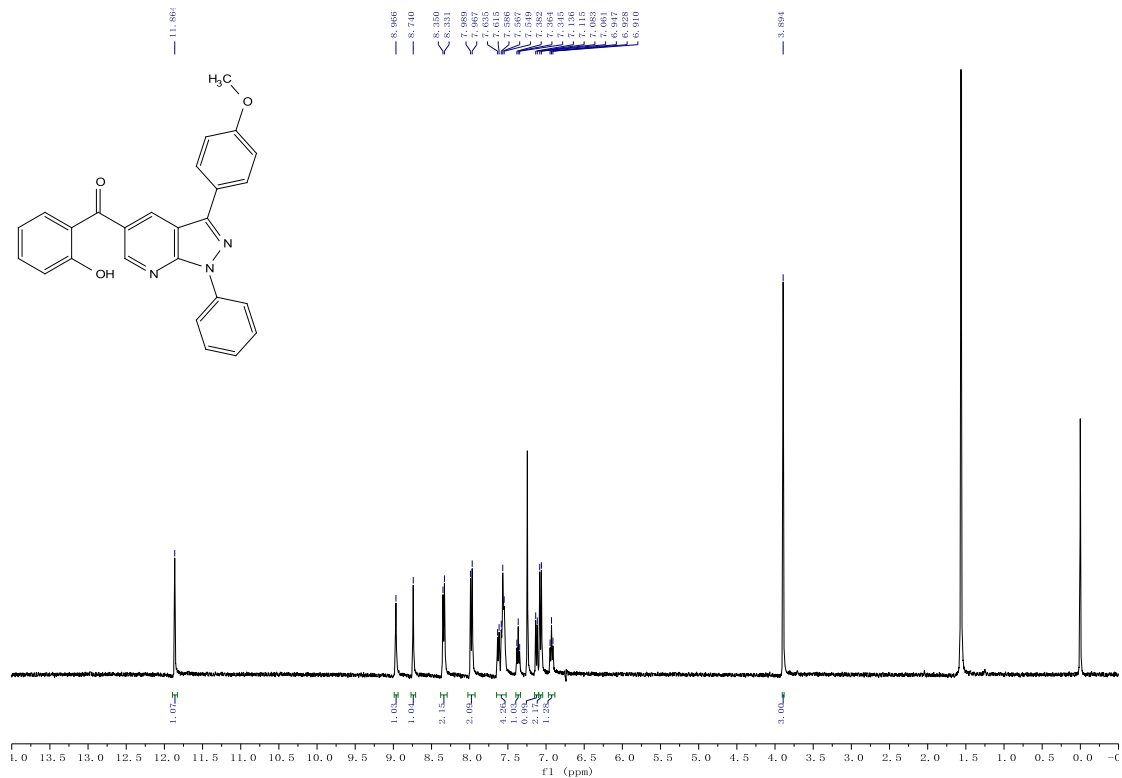
(3b).



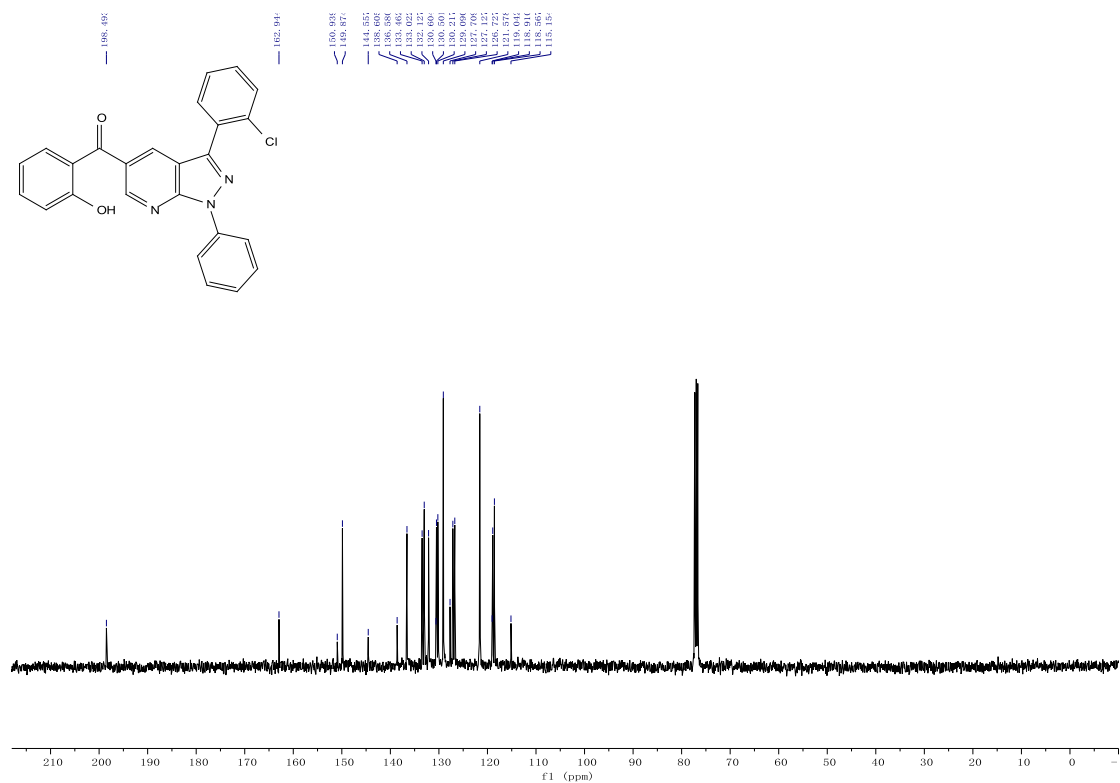
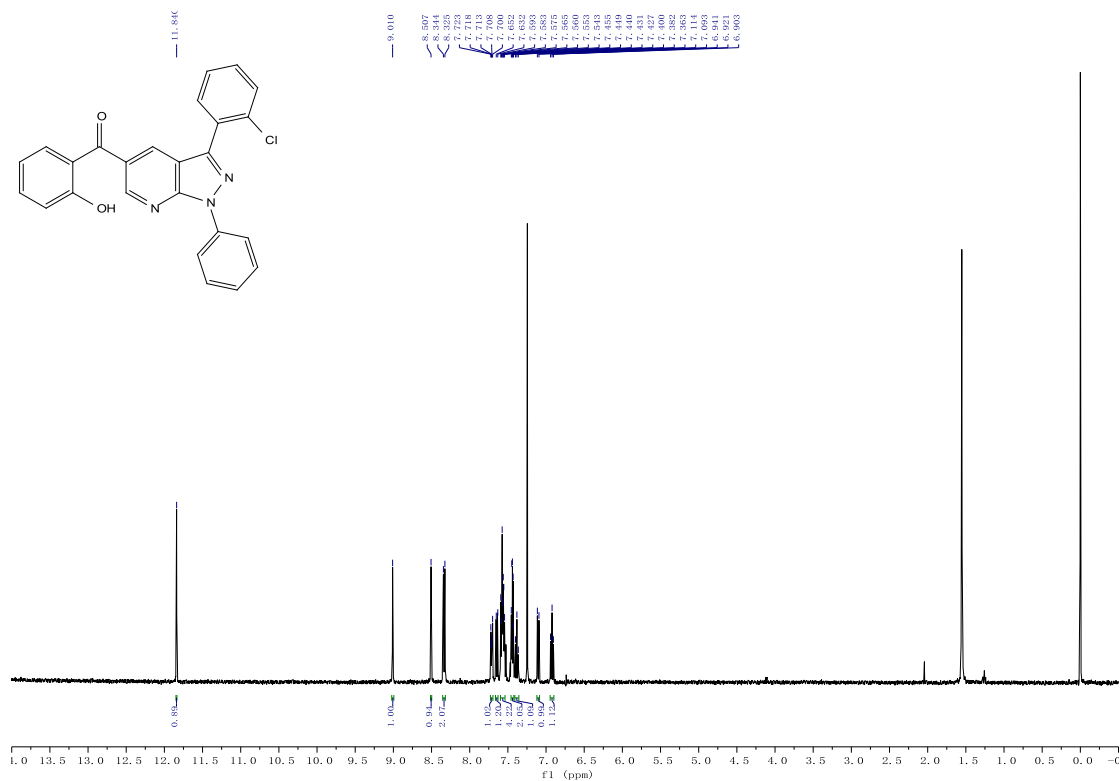
**(5-chloro-2-hydroxyphenyl)(1-phenyl-3-(p-tolyl)-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (3c).**



**(2-hydroxyphenyl)(3-(4-methoxyphenyl)-1-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (3d).**

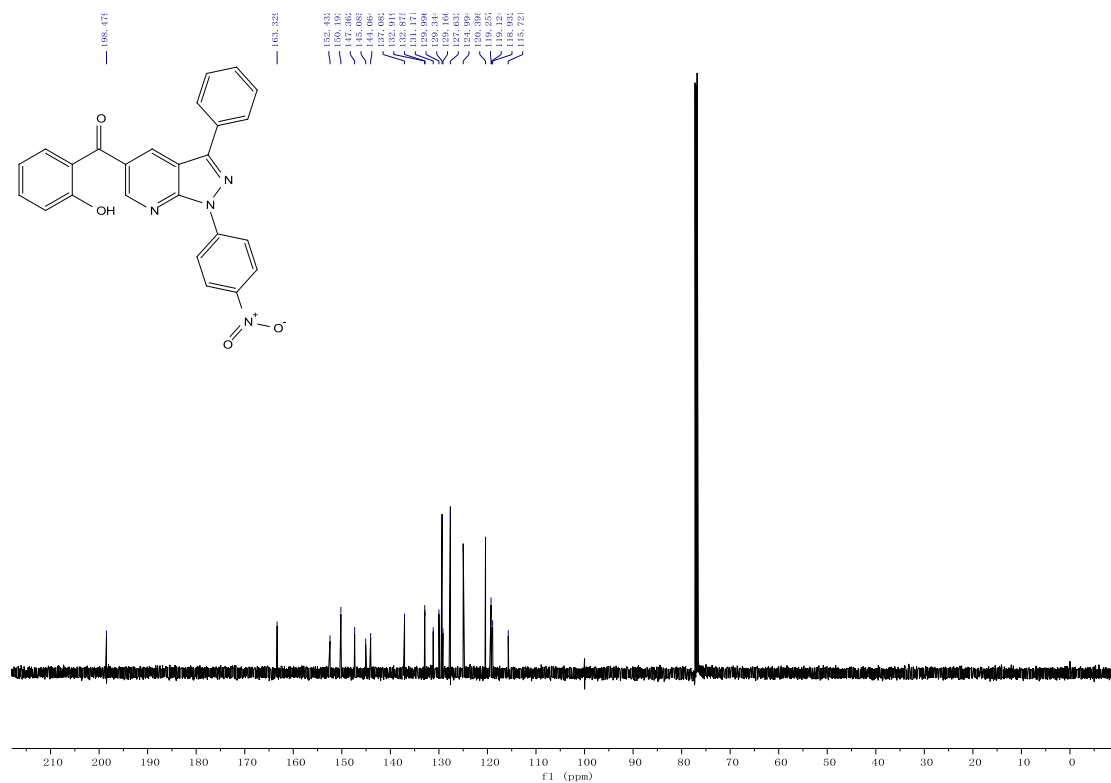
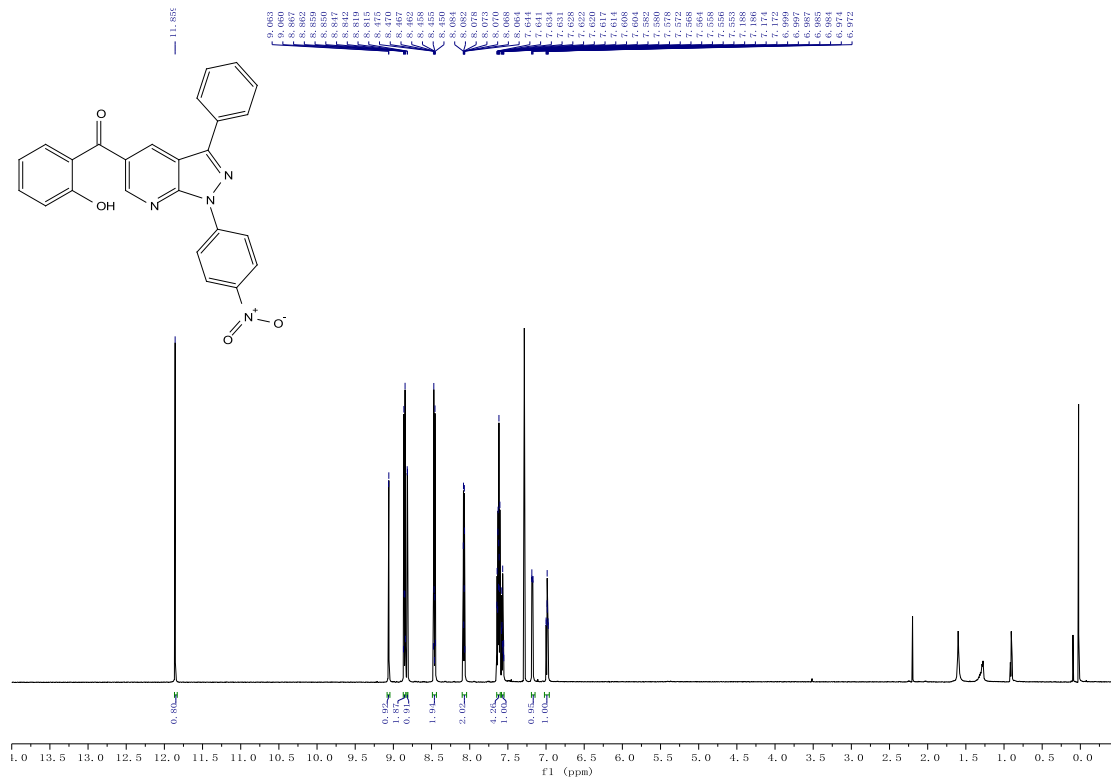


**(3-(2-chlorophenyl)-1-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)(2-hydroxyphenyl)methanone (3e).**



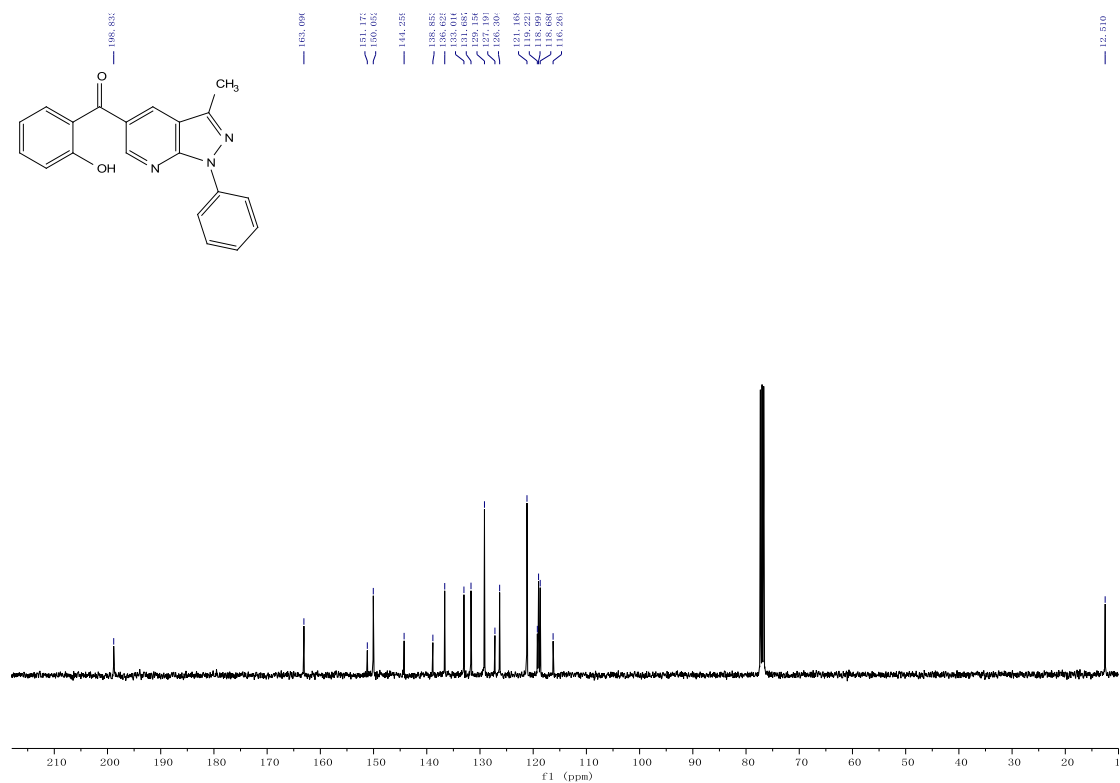
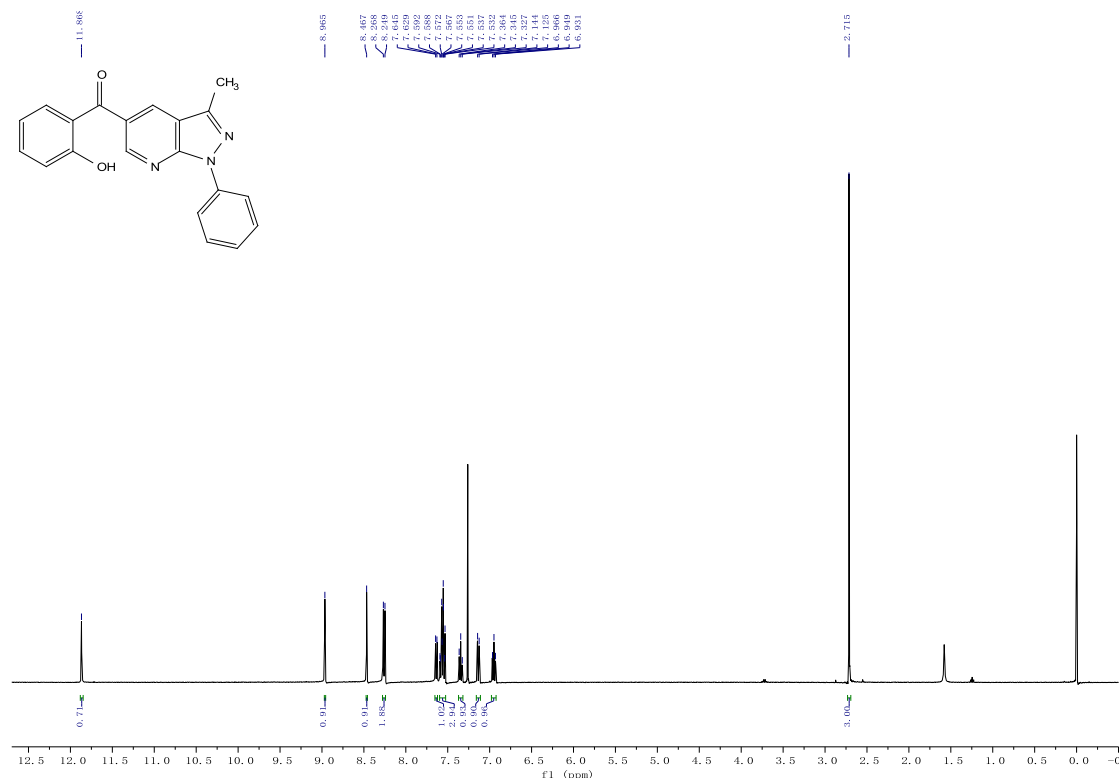


**(2-hydroxyphenyl)(1-(4-nitrophenyl)-3-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (3g).**

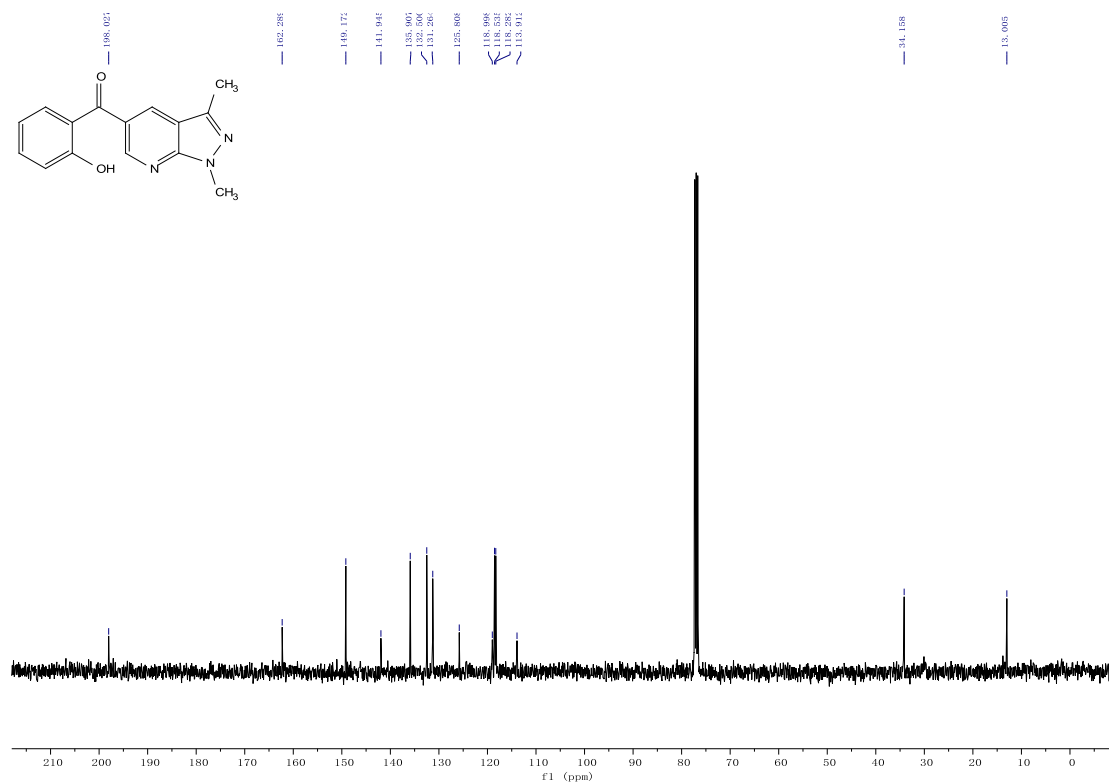
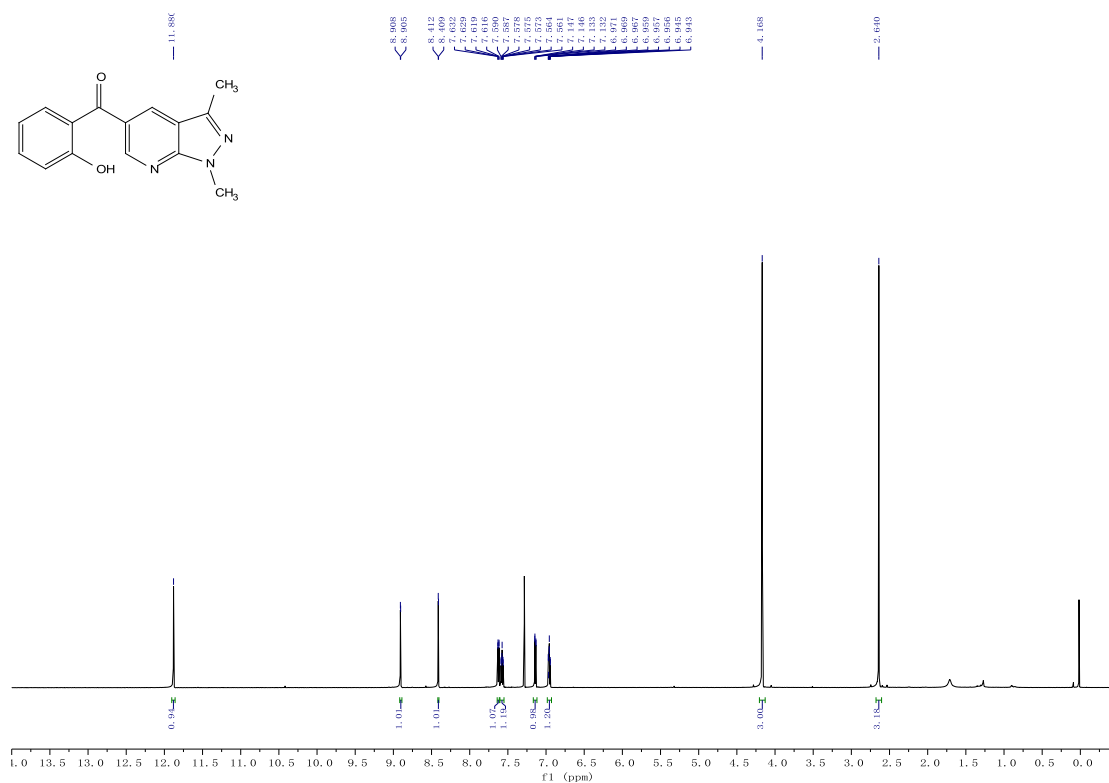


(2-hydroxyphenyl)(3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone

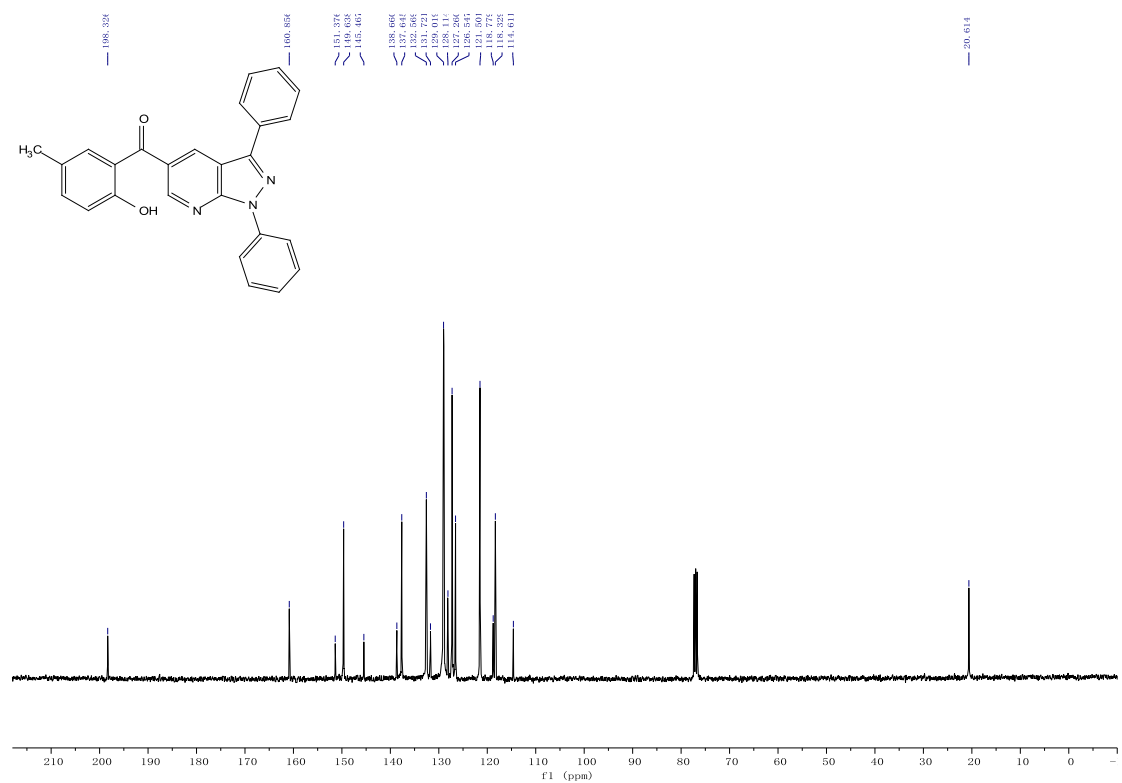
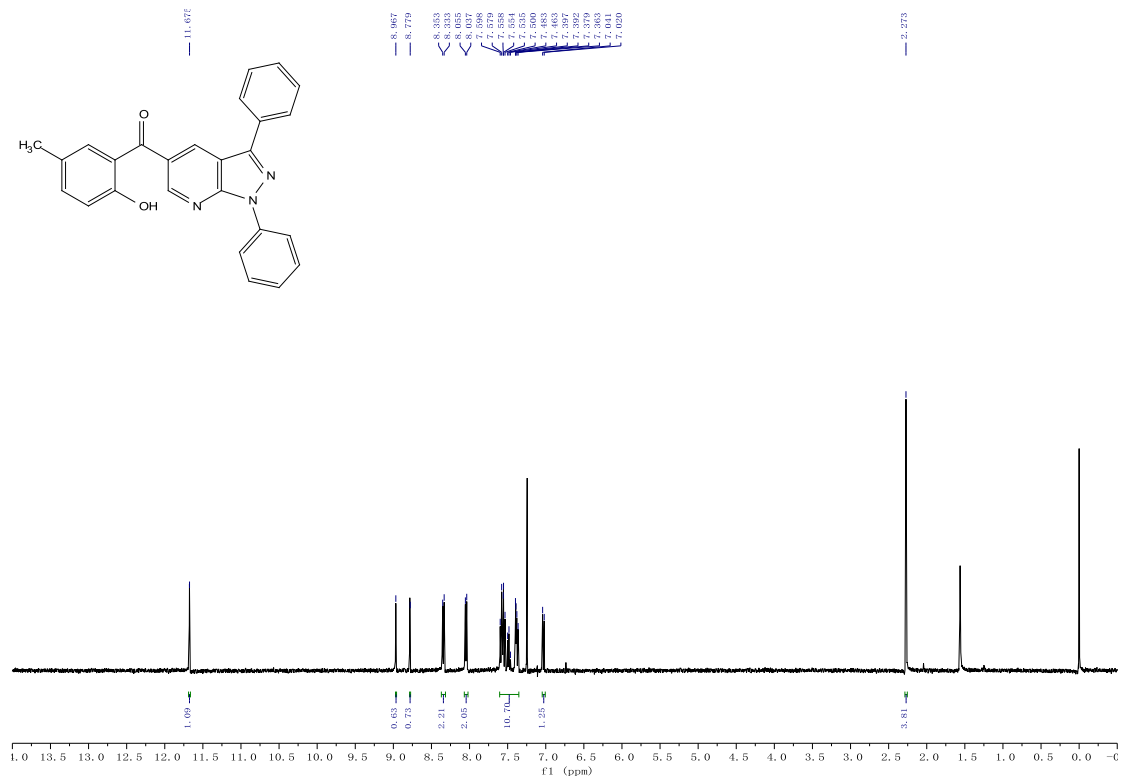
(3h).



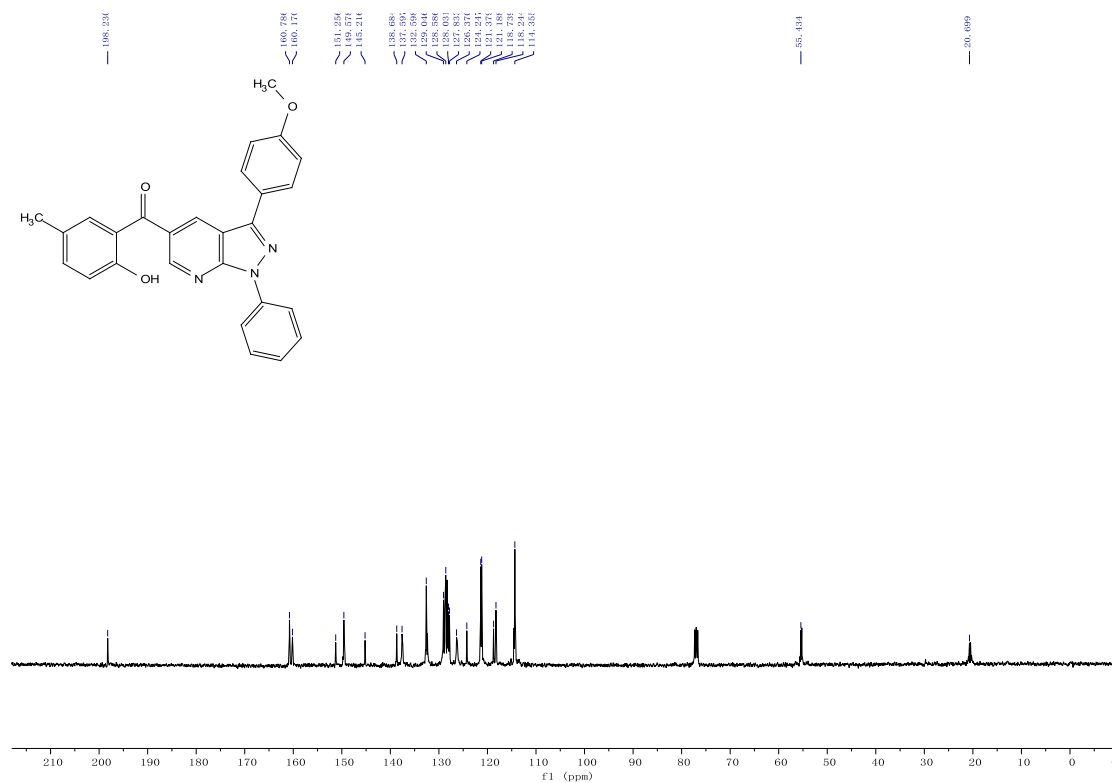
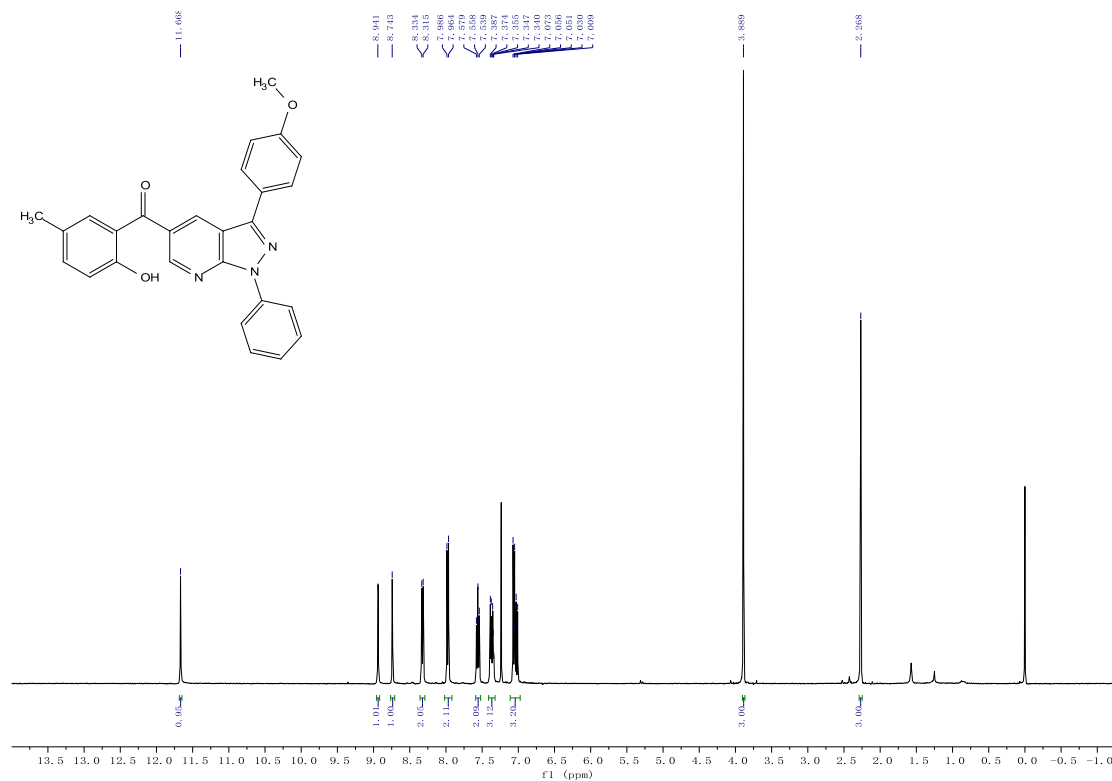
**(1,3-dimethyl-1H-pyrazolo[3,4-b]pyridin-5-yl)(2-hydroxyphenyl)methanone (3i).**



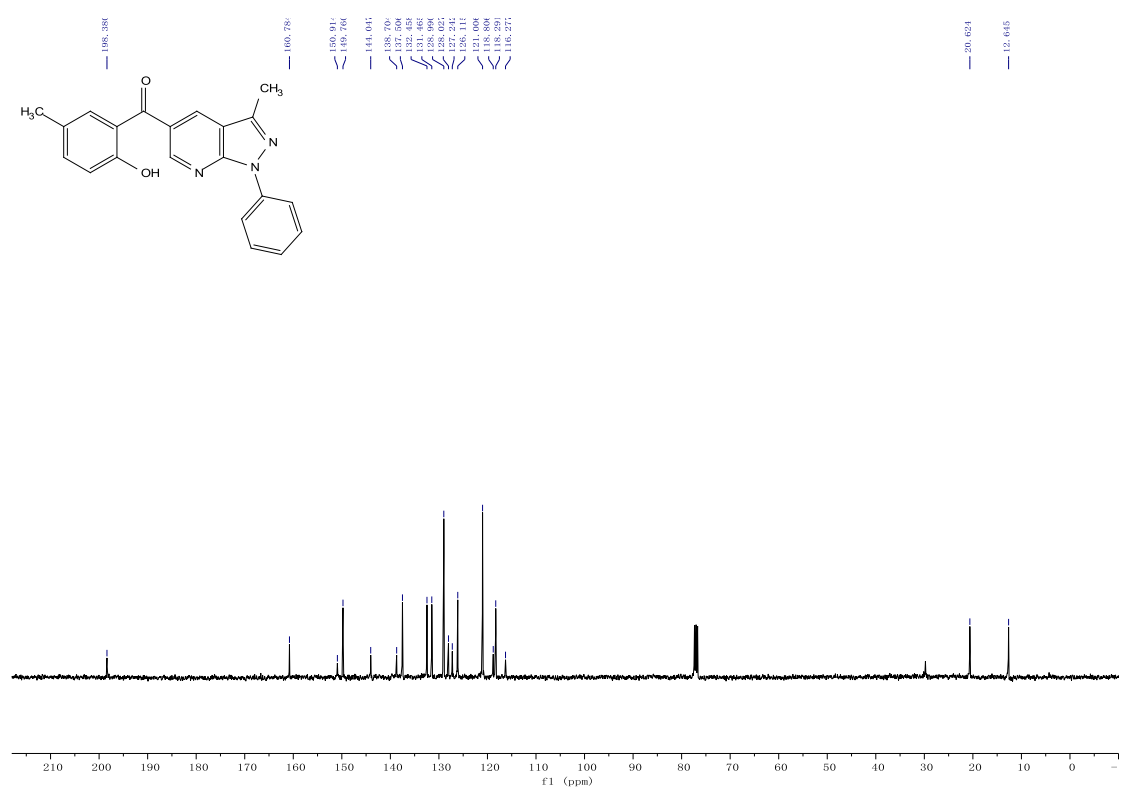
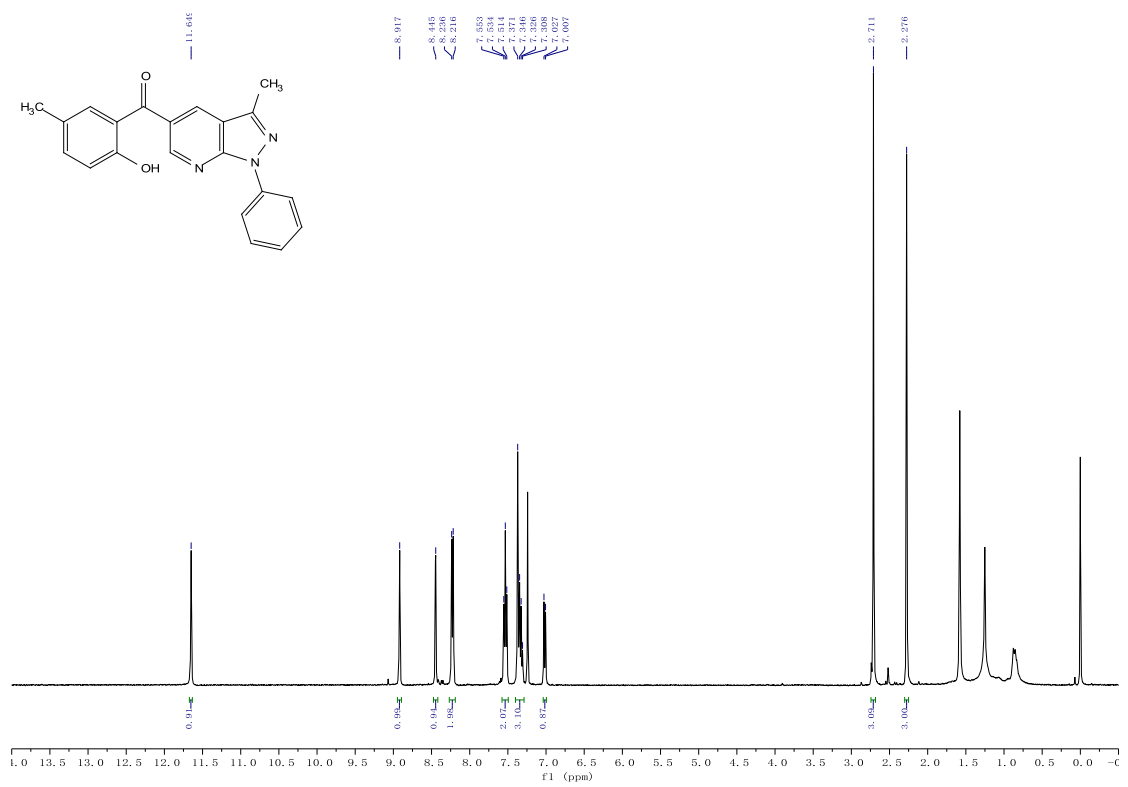
**(1,3-diphenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)(2-hydroxy-5-methylphenyl)methanone**  
**(3j).**



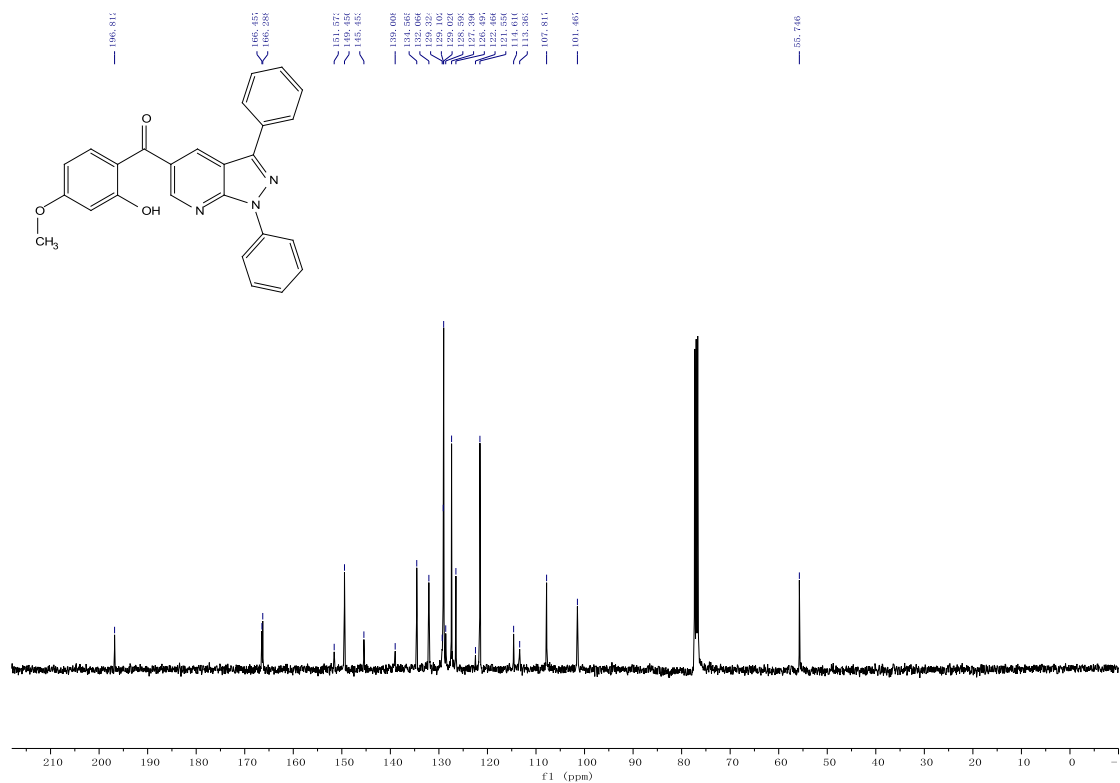
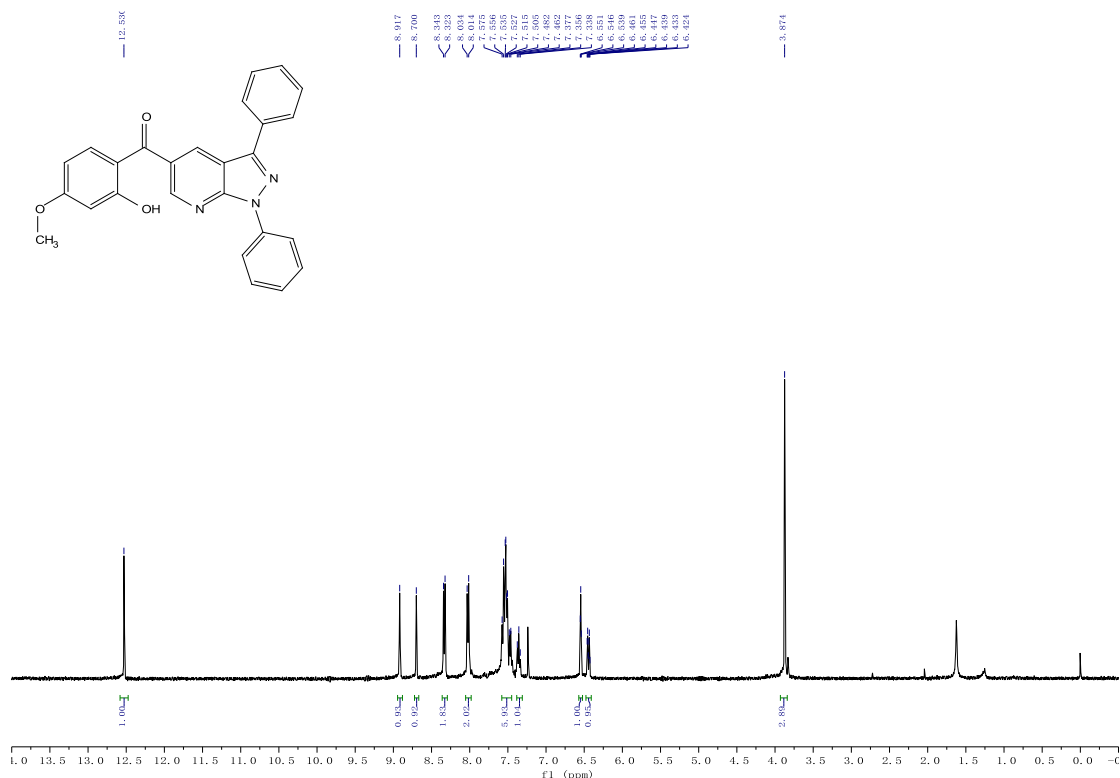
**(2-hydroxy-5-methylphenyl)(3-(4-methoxyphenyl)-1-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (3k).**



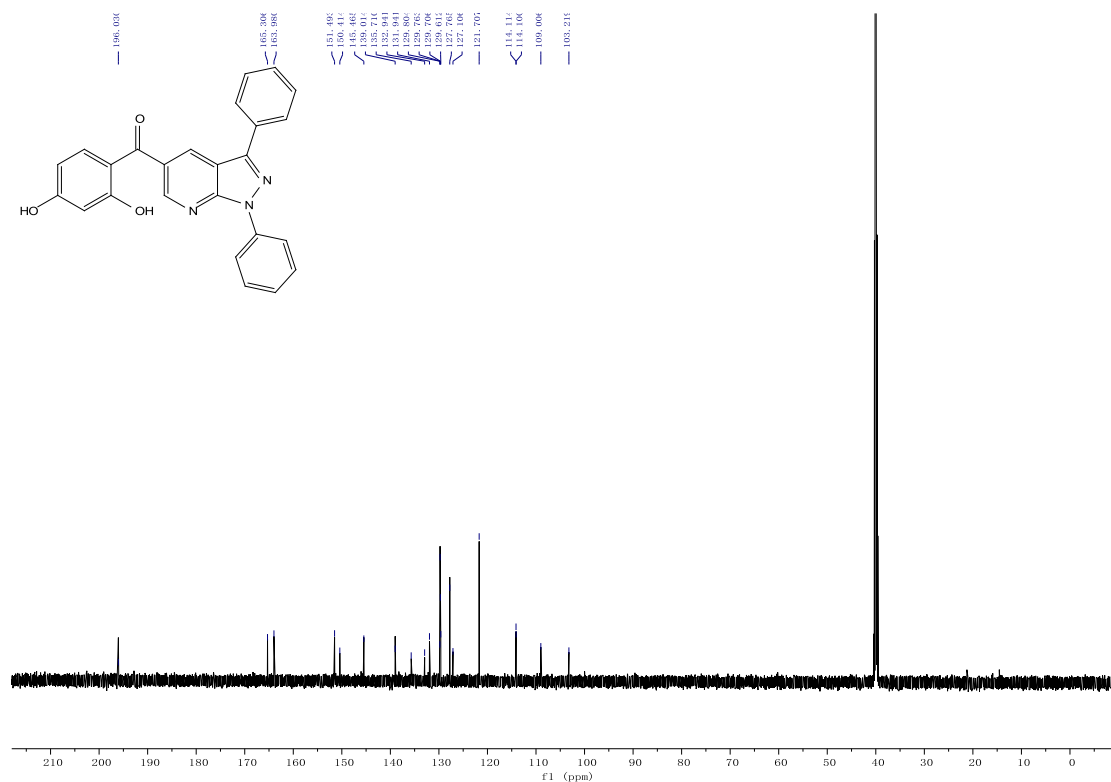
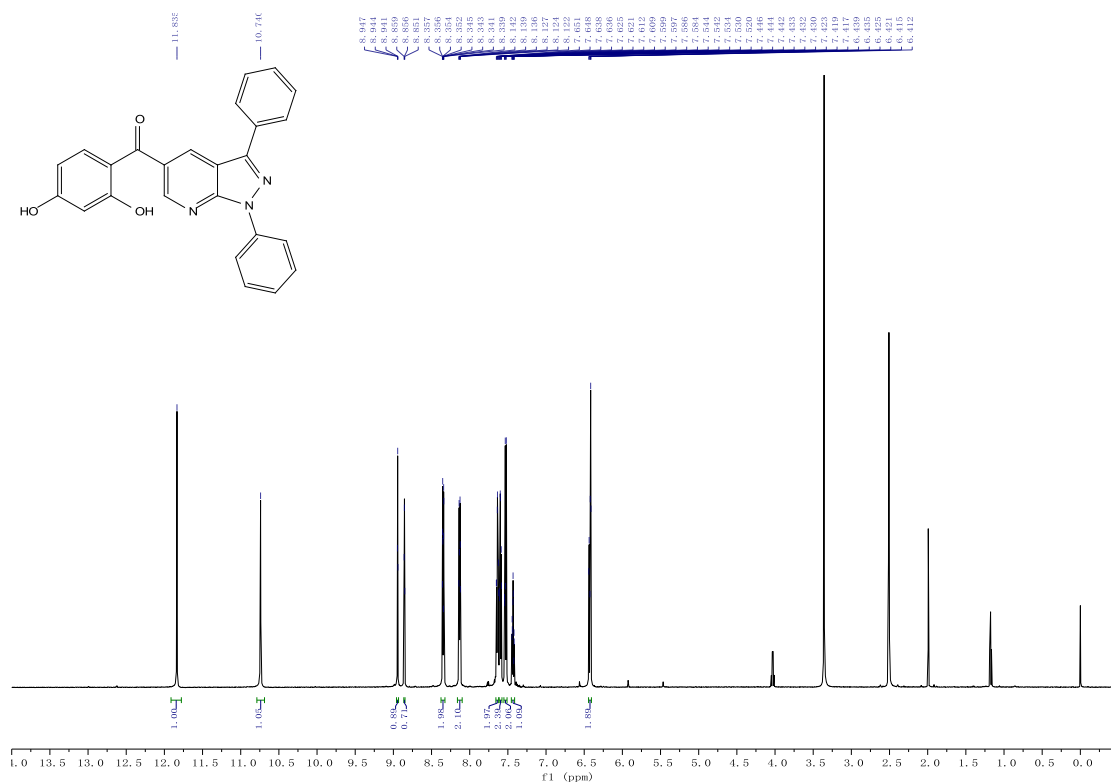
**(2-hydroxy-5-methylphenyl)(3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (3l).**



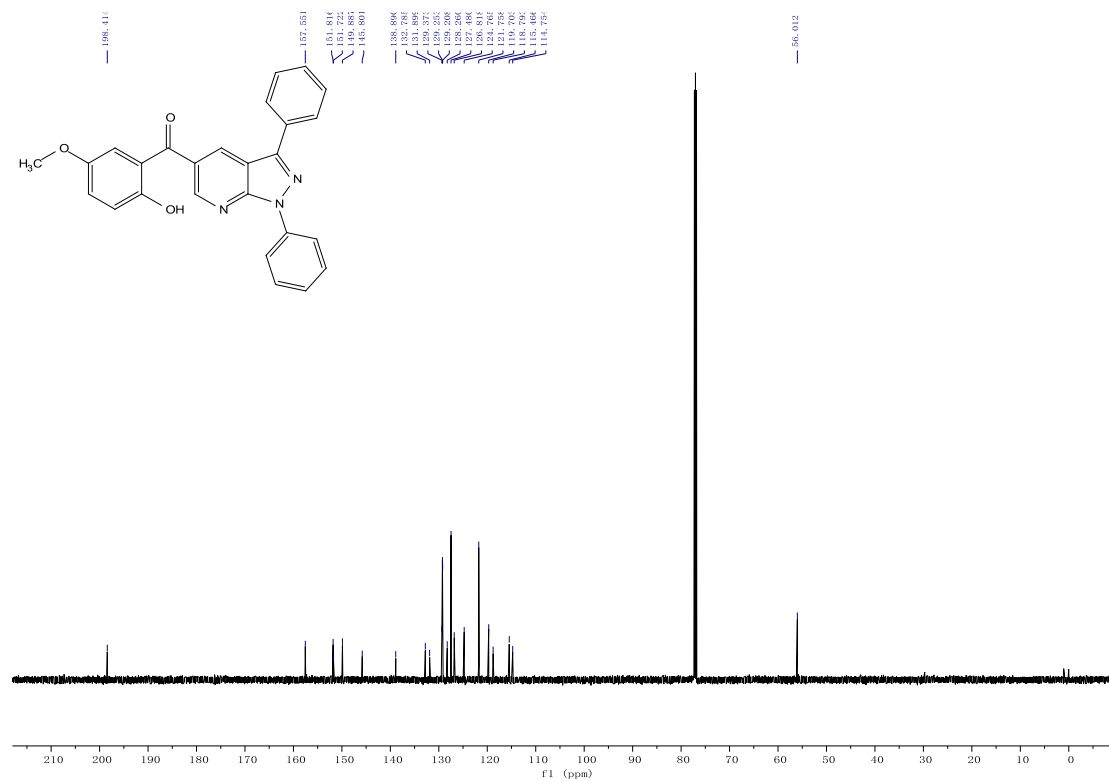
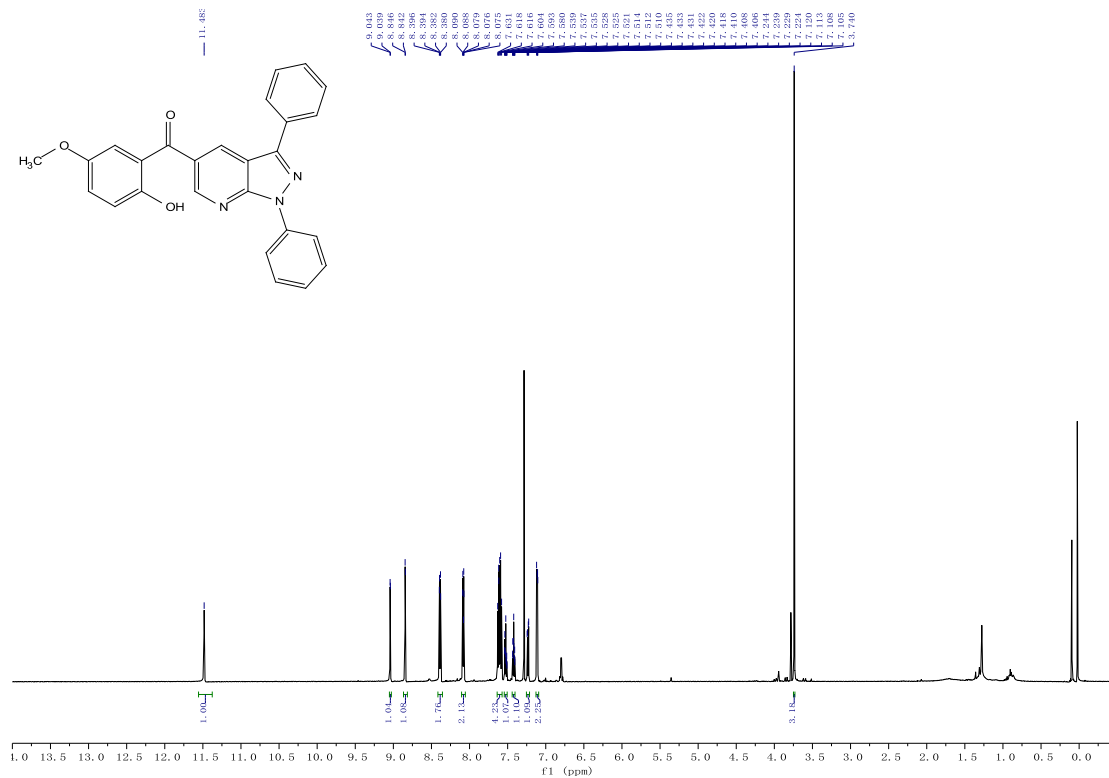
**(1,3-diphenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)(2-hydroxy-4-methoxyphenyl)methanone (3m).**



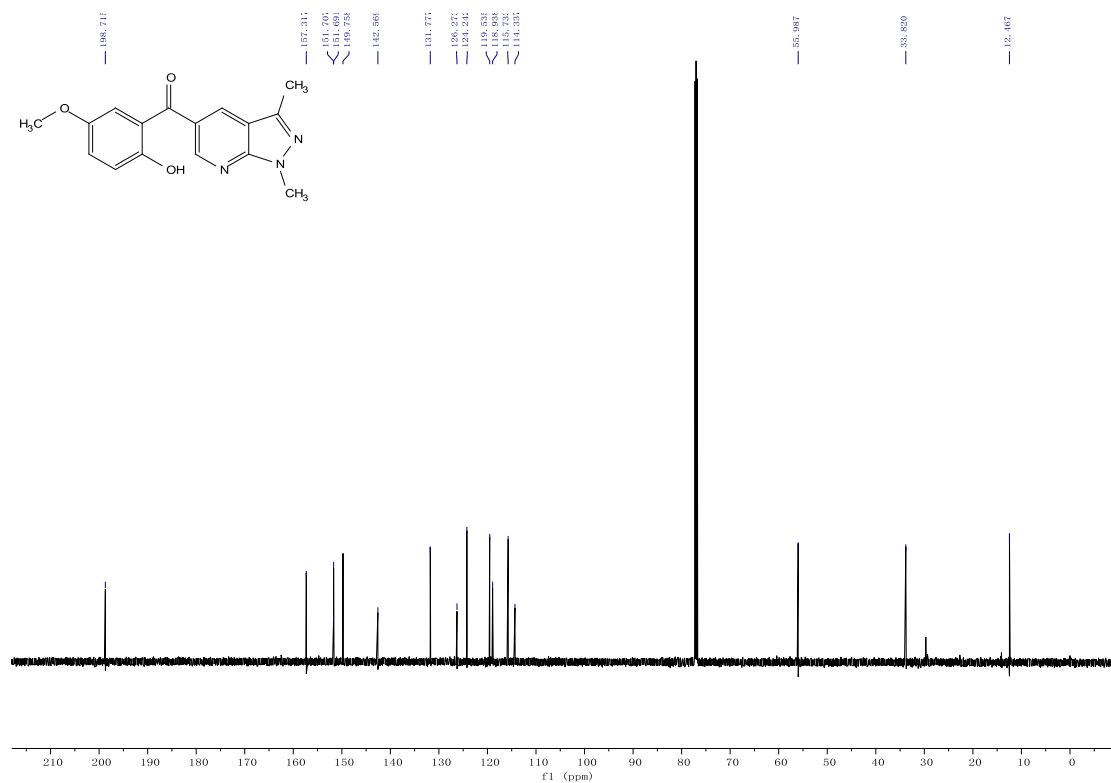
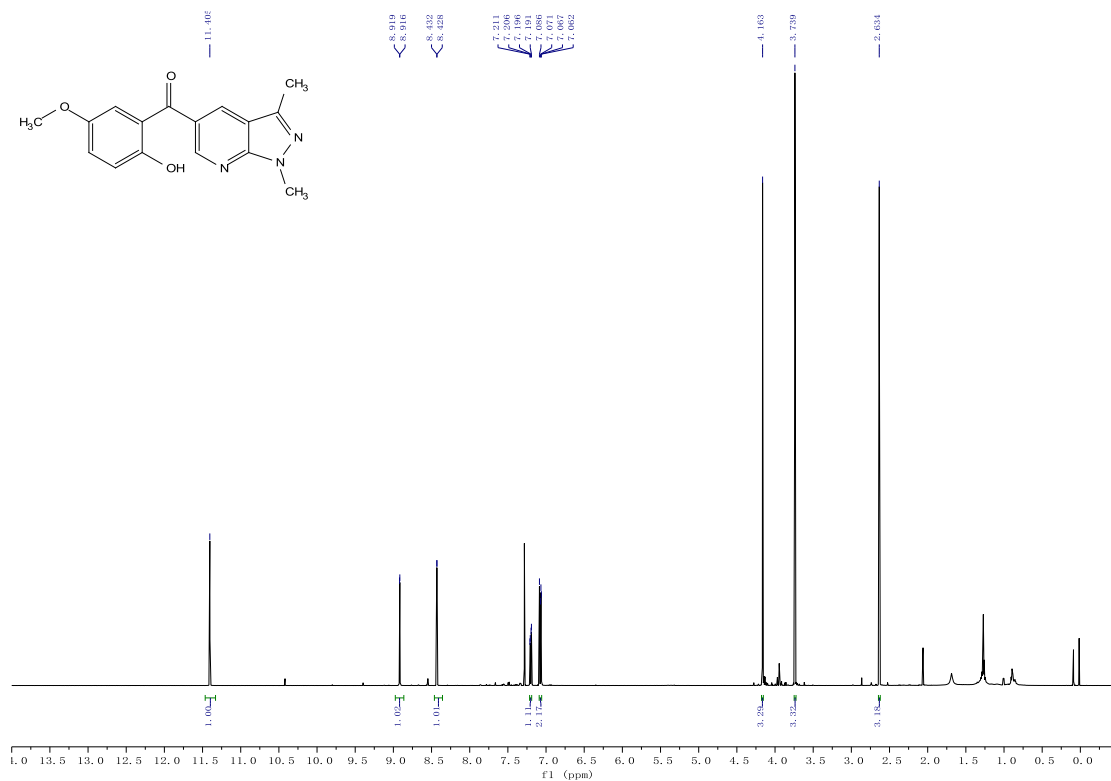
(2,4-dihydroxyphenyl)(1,3-diphenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (3n).



**(1,3-diphenyl-1*H*-pyrazolo[3,4-*b*]pyridin-5-yl)(2-hydroxy-5-methoxyphenyl)methanone (3o).**

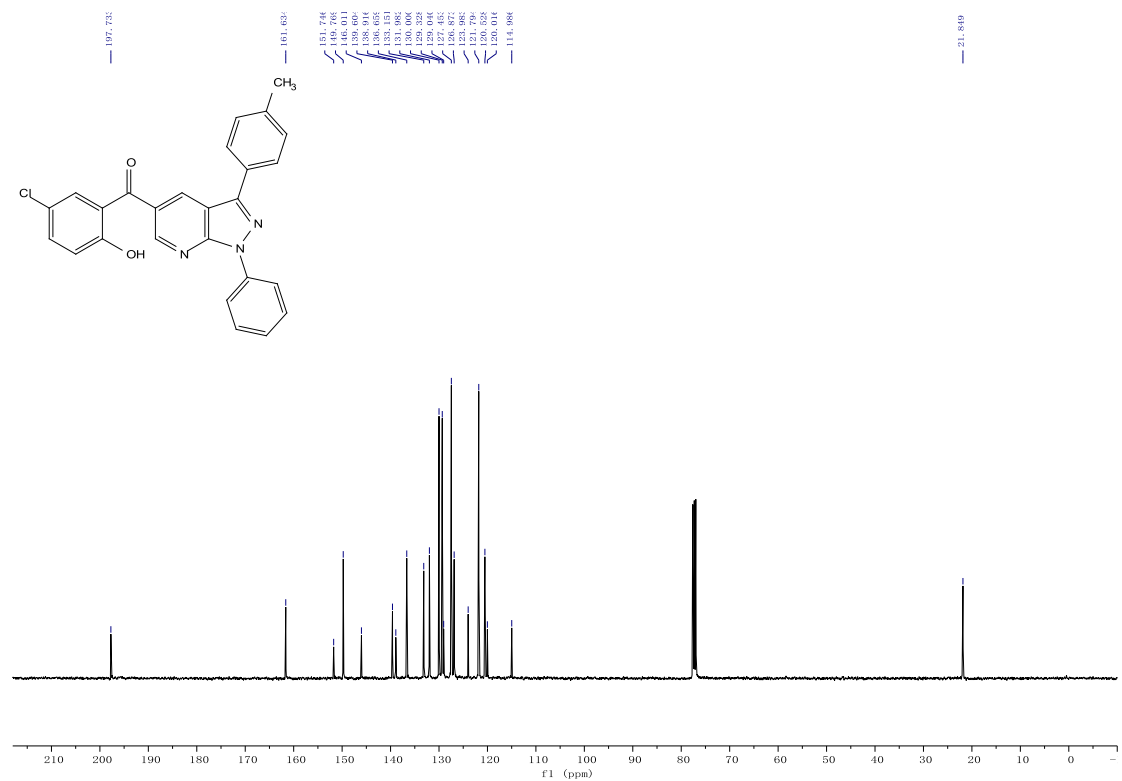
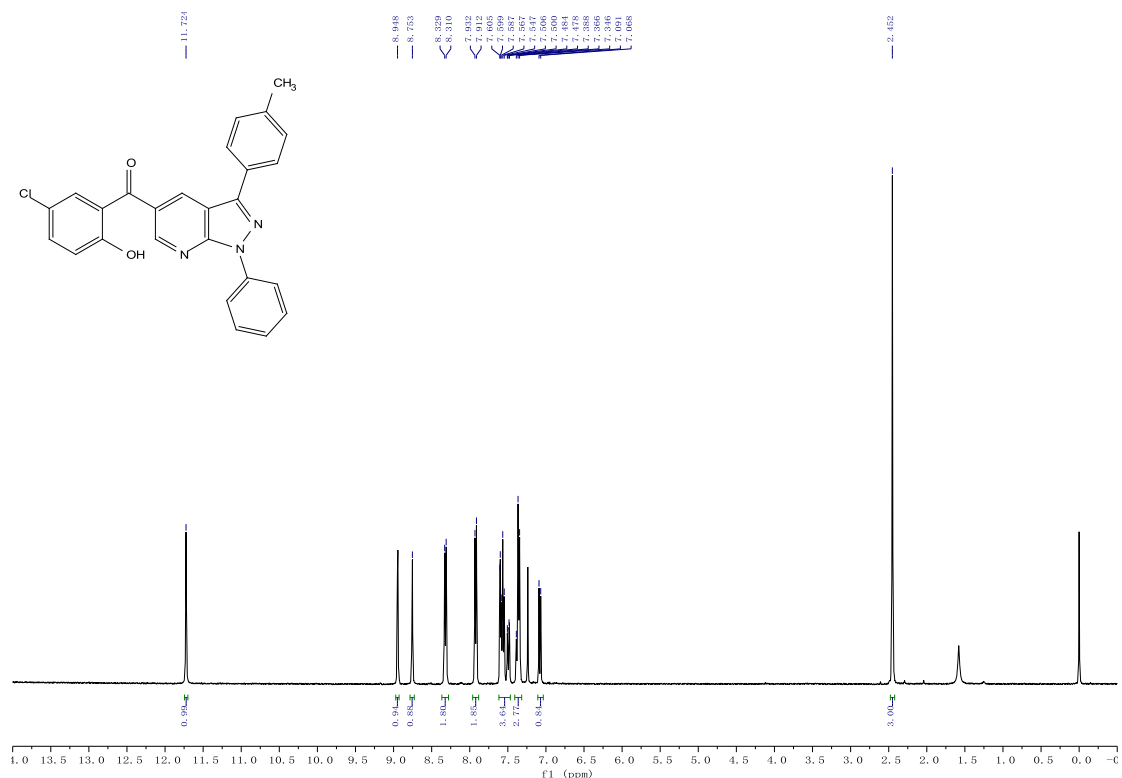


**(1,3-dimethyl-1*H*-pyrazolo[3,4-*b*]pyridin-5-yl)(2-hydroxy-5-methoxyphenyl)methanone (3p).**

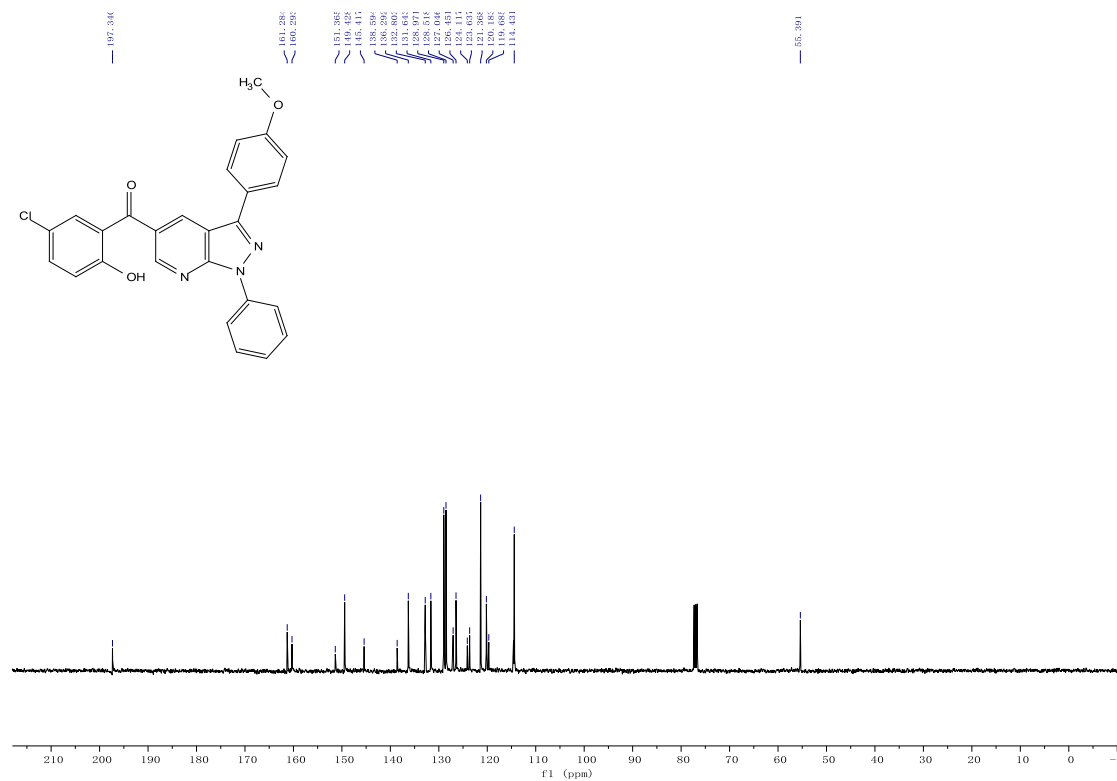
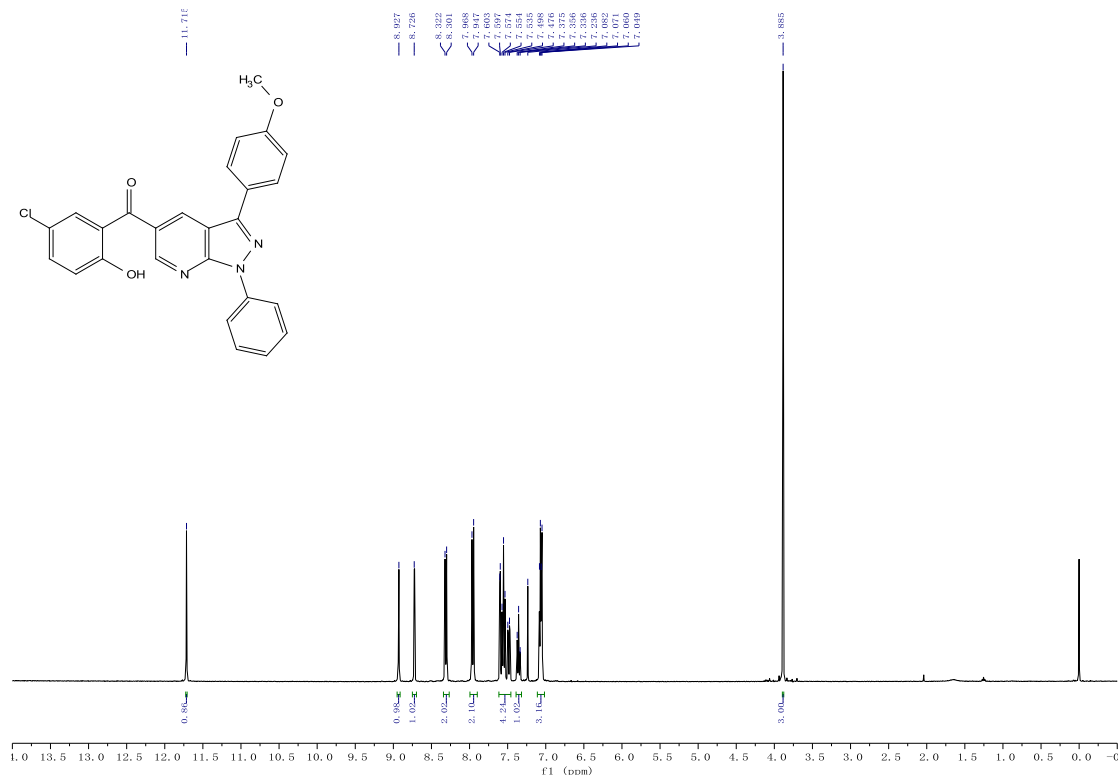




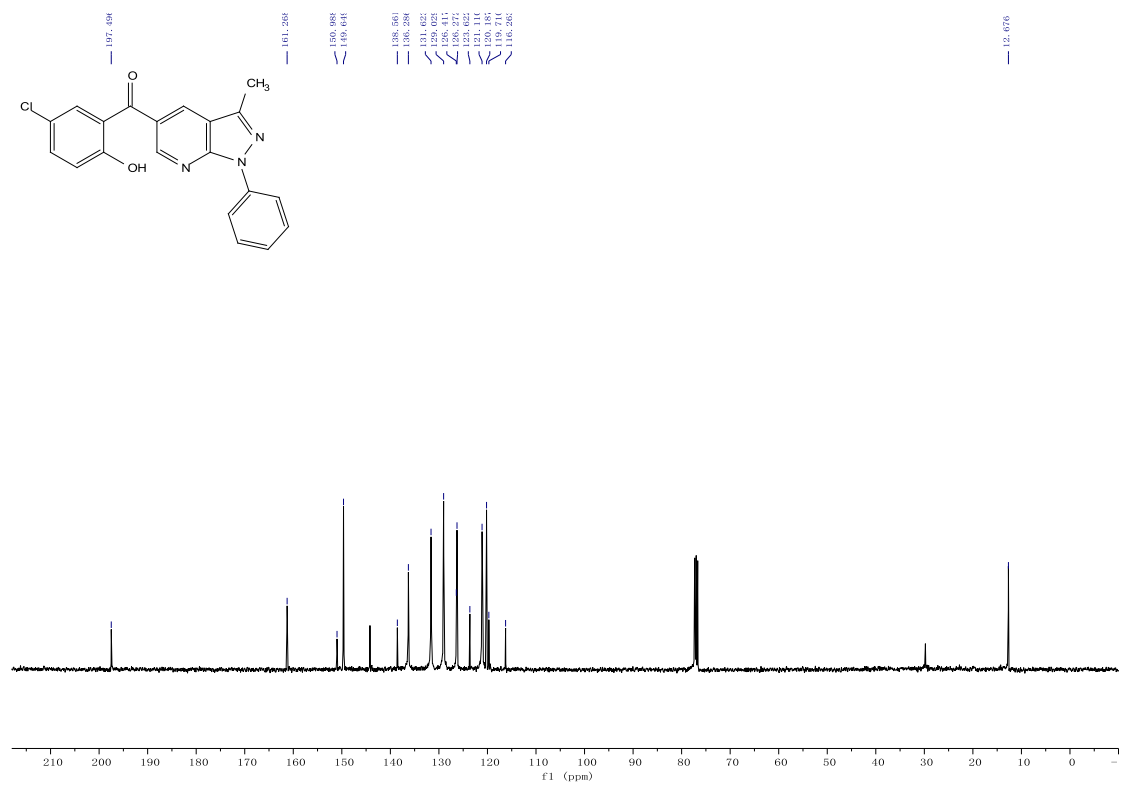
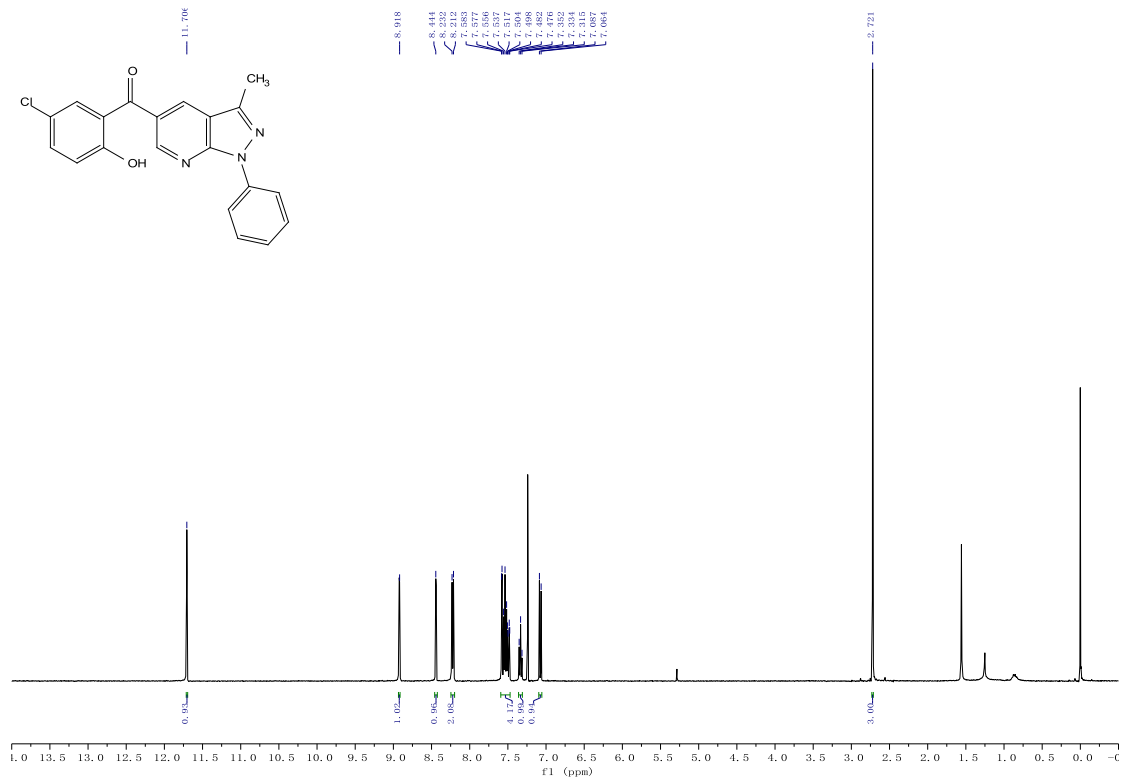
**(5-chloro-2-hydroxyphenyl)(1-phenyl-3-(p-tolyl)-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (3r).**



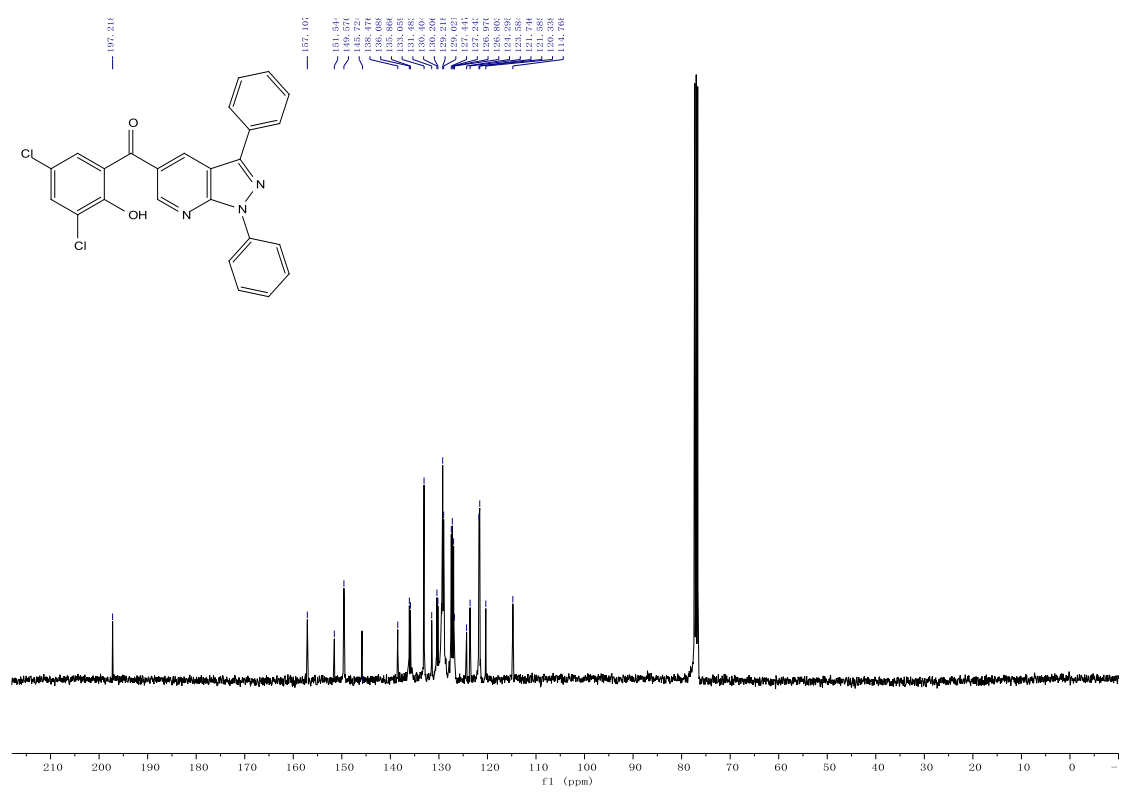
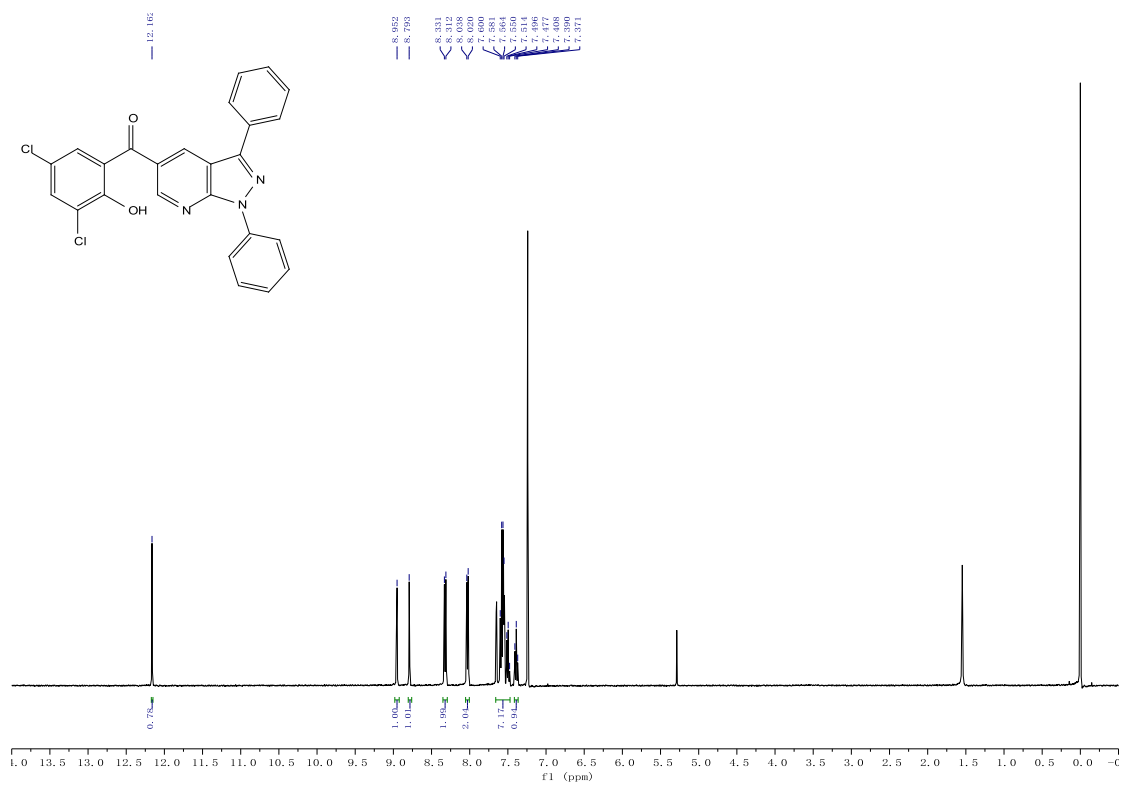
**(5-chloro-2-hydroxyphenyl)(3-(4-methoxyphenyl)-1-phenyl-1H-pyrazolo[3,4-b]pyridi  
n-5-yl)methanone (3s).**



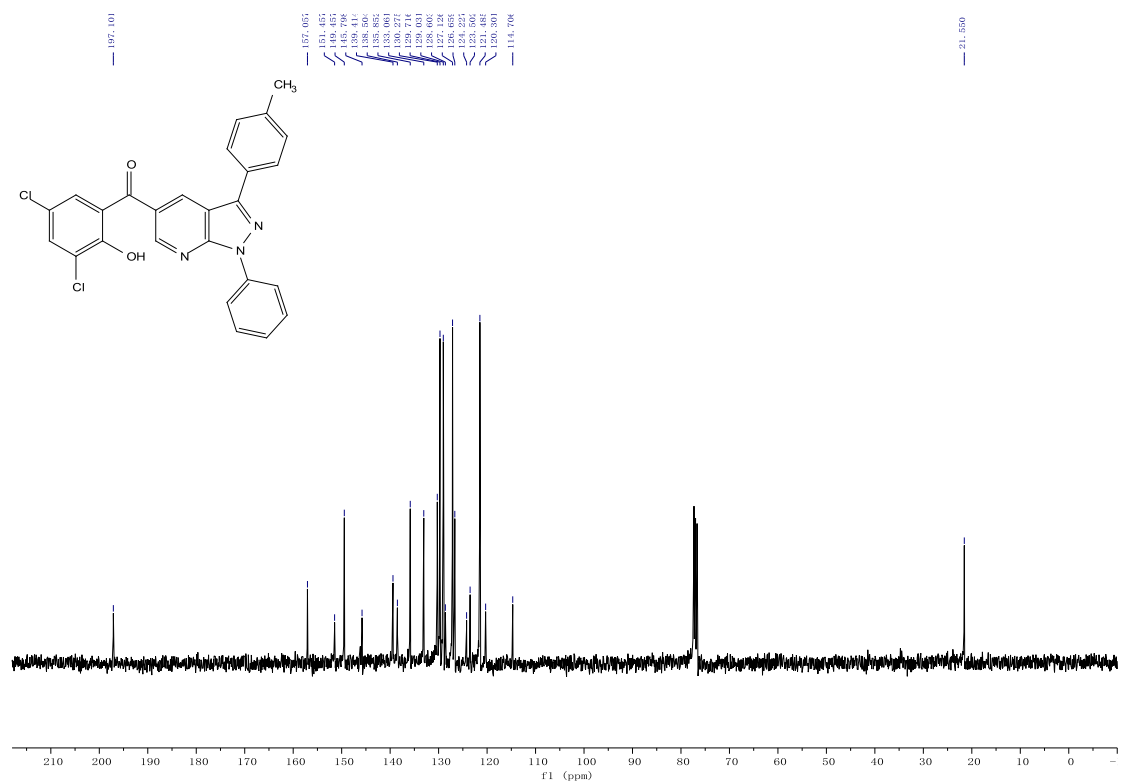
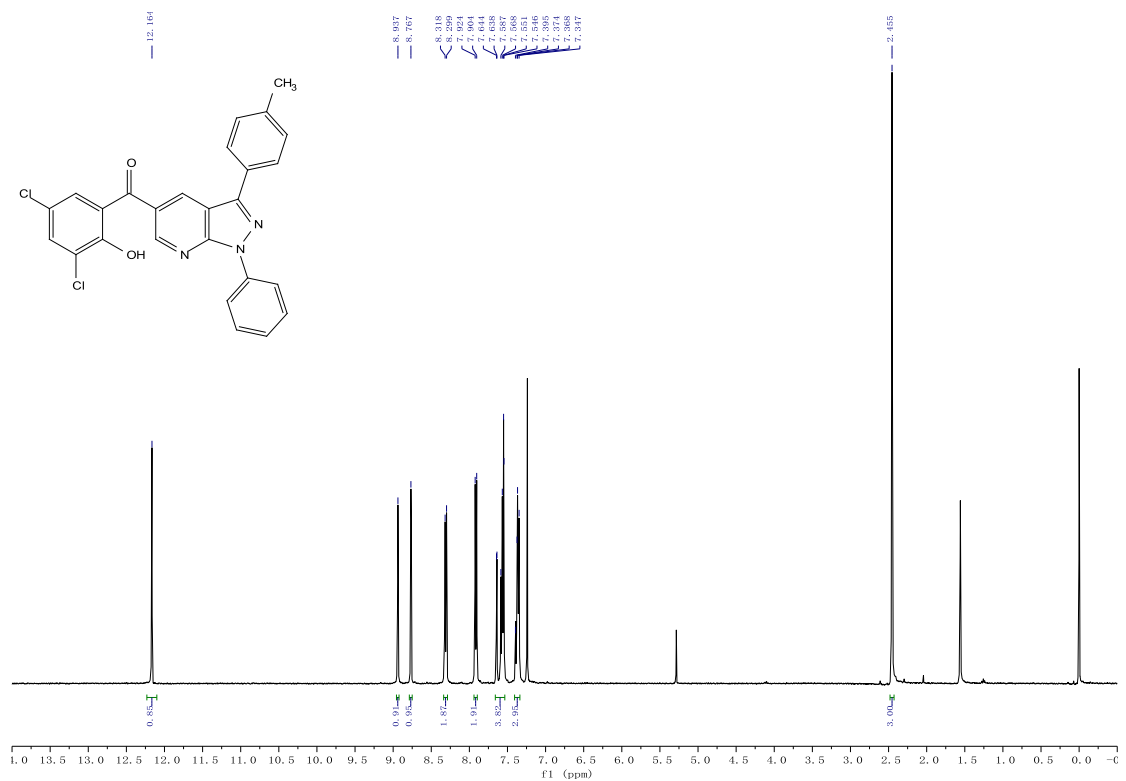
**(5-chloro-2-hydroxyphenyl)(3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (3t).**



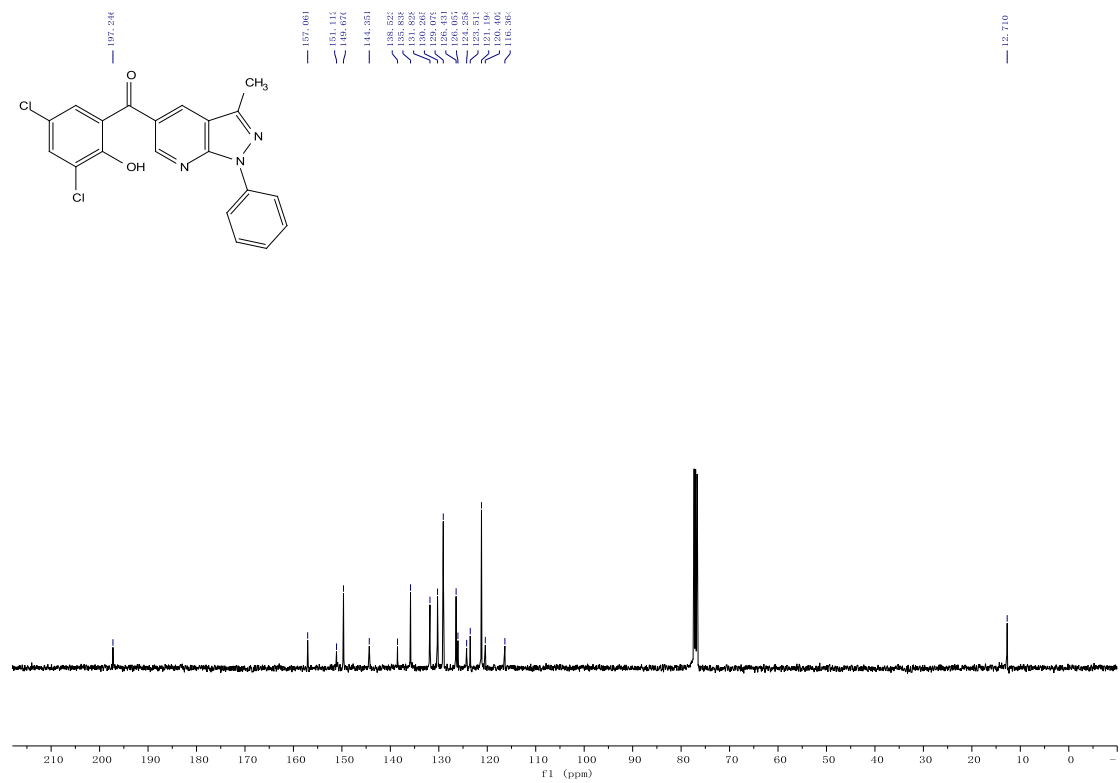
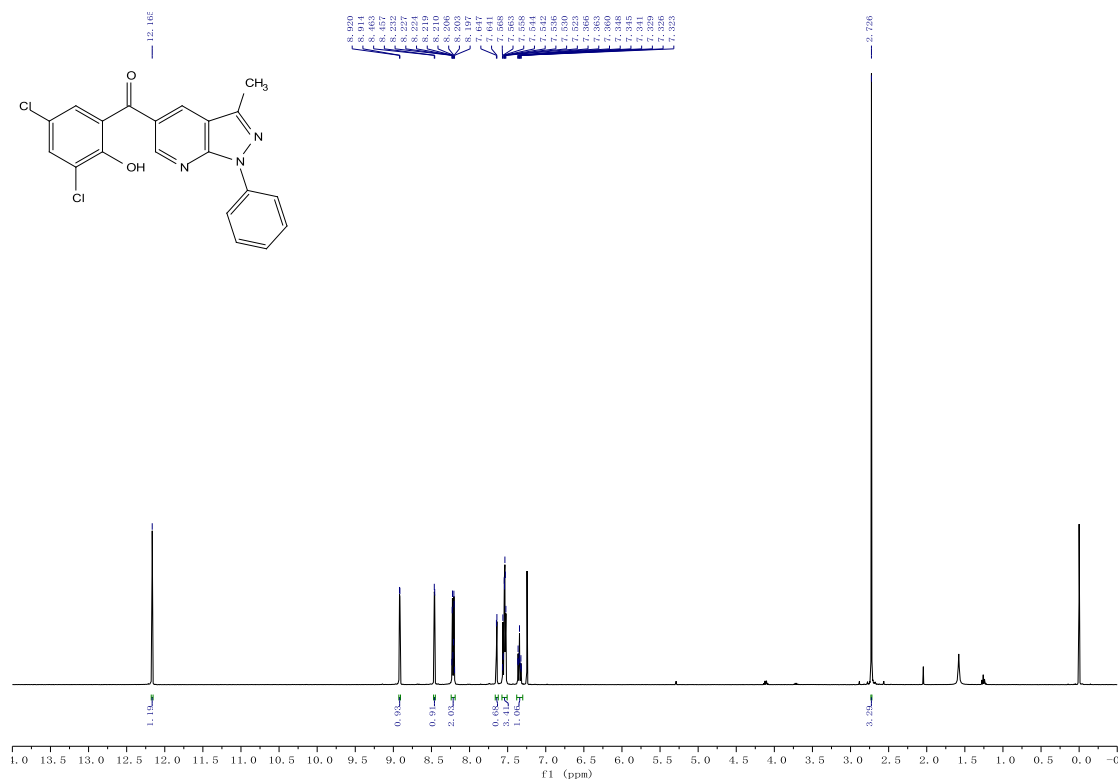
**(3,5-dichloro-2-hydroxyphenyl)(1,3-diphenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (3u).**



**(3,5-dichloro-2-hydroxyphenyl)( 1-phenyl-3-(p-tolyl)-1H-pyrazolo[3,4-b]pyridin-5-yl)  
methanone (3v)**

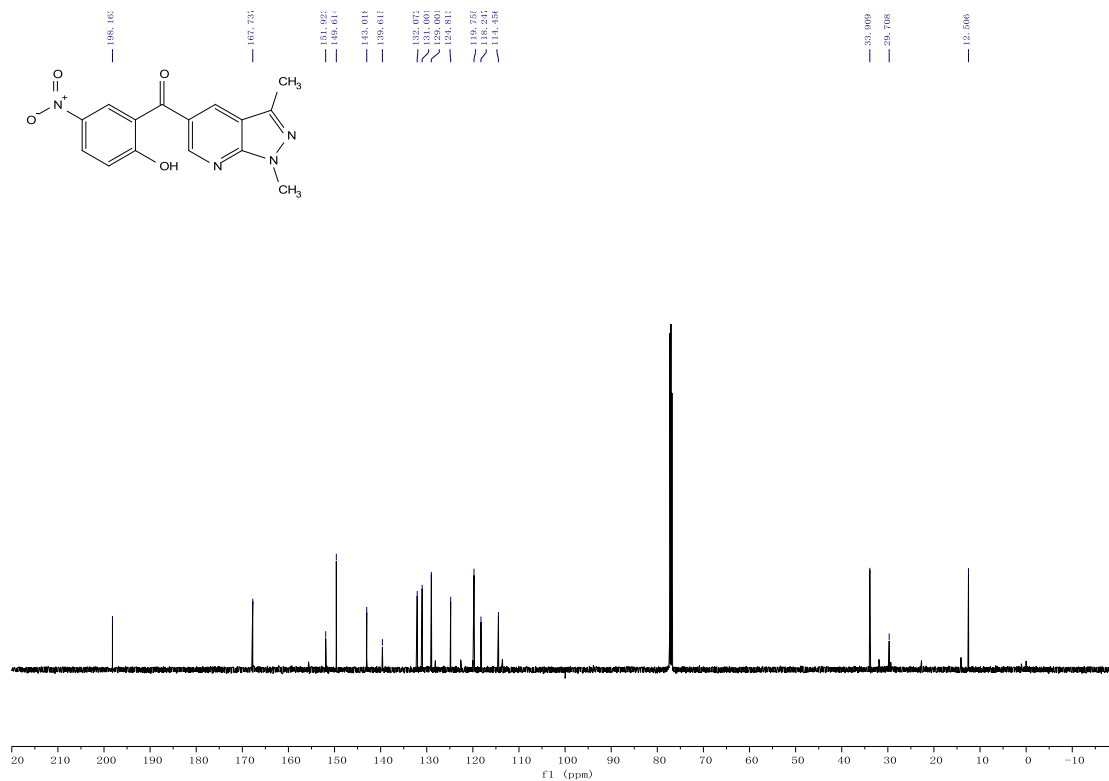
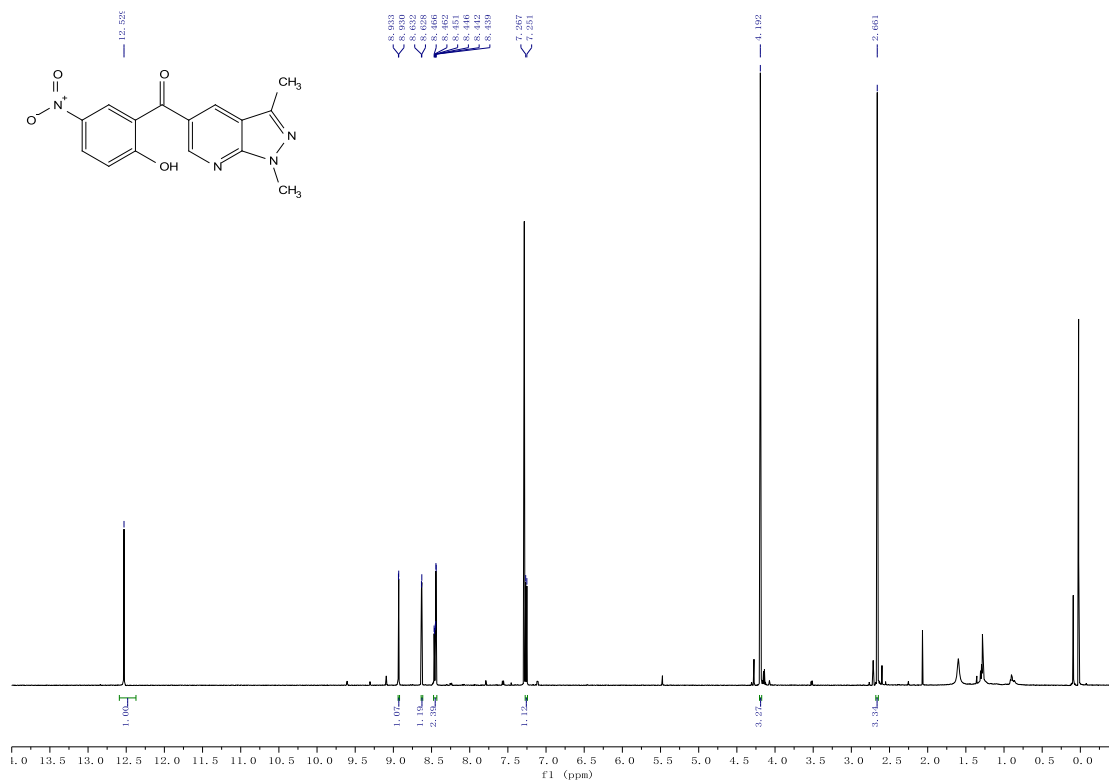


**(3,5-dichloro-2-hydroxyphenyl)(3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)methanone (3w)**



# (1,3-dimethyl-1H-pyrazolo[3,4-b]pyridin-5-yl)(2-hydroxy-5-nitrophenyl)methanone

(3x)



(1,3-diphenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)(2-hydroxy-5-nitrophenyl)methanone

(3y).

