Supporting Information

One-Pot NBS-Promoted Synthesis of Imidazoles and Thiazoles from Ethylarenes in Water

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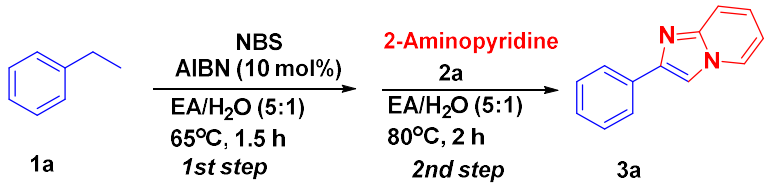
Contents

(A) Optimization of reaction conditions.

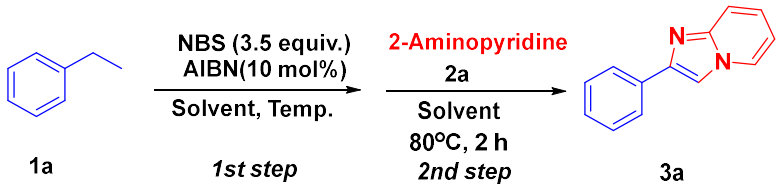
Table S1. Optimization of equivalents of oxidant[a]



First step			Second step			
Entry.	**Oxidant (equiv.)**	**Solvent**	**Solvent**	**Temp. (°C)**	**Base (equiv.)**	**Yield[b] (%)**
1	NBS (3.5)	EA/H2O (5:1)	EA/H2O (5:1)	80	none	38
2	NBS (2.5)	EA/H2O (5:1)	EA/H2O (5:1)	80	none	27
3	NBS (4.5)	EA/H2O (5:1)	EA/H2O (5:1)	80	none	36

[a] Reactions were run with ethylbenzene **1a** (1 mmol) of with NBS in the presence of AIBN (10 mol%) in EA:H2O (5:1, 6 mL) at 65 °C for 1.5 h, followed by reaction with 2-aminopyridine **2a** (1.2 mmol) at 80°C for 2 h. [b] Isolated yields.

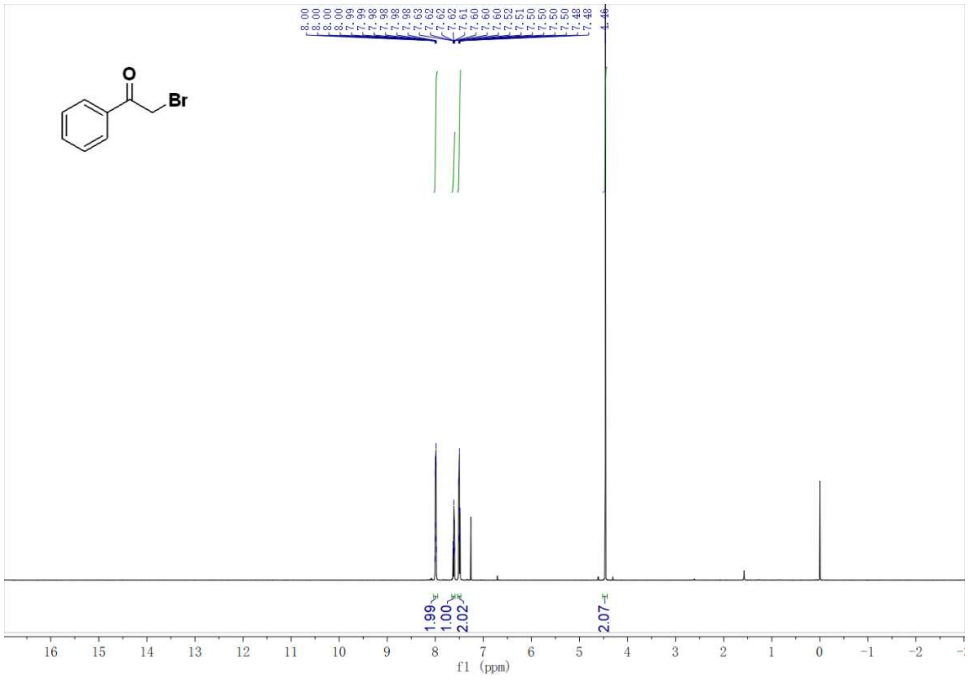
Table S2. Optimization of solvent and temperature of first step[a]

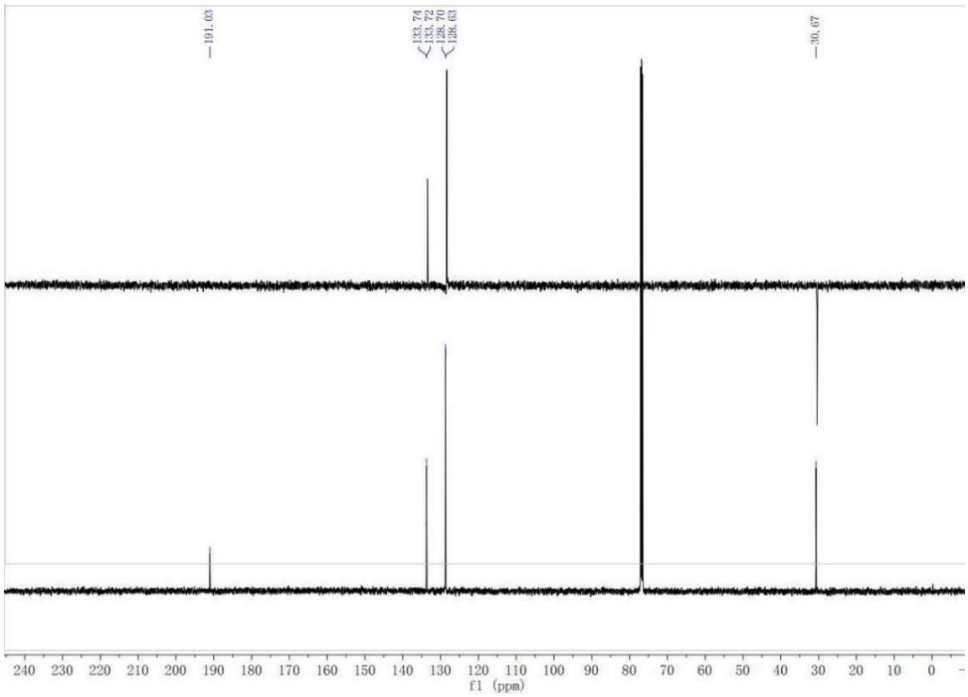


First step				Second step			
Entry.	Oxidant	Solvent	Temp. (°C)	Solvent	Temp. (°C)	Base (equiv.)	Yield[b] (%)
1	NBS	EA/H2O (5:1)	65	EA/H2O (5:1)	80	none	38
2	NBS	EA/H2O (10:1)	65	EA/H2O (10:1)	80	none	36
3	NBS	EA/H2O (2:1)	65	EA/H2O (2:1)	80	none	23
4	NBS	EA/H2O (5:1)	60	EA/H2O (5:1)	80	none	35
5	NBS	EA/H2O (5:1)	70	EA/H2O (5:1)	80	none	28

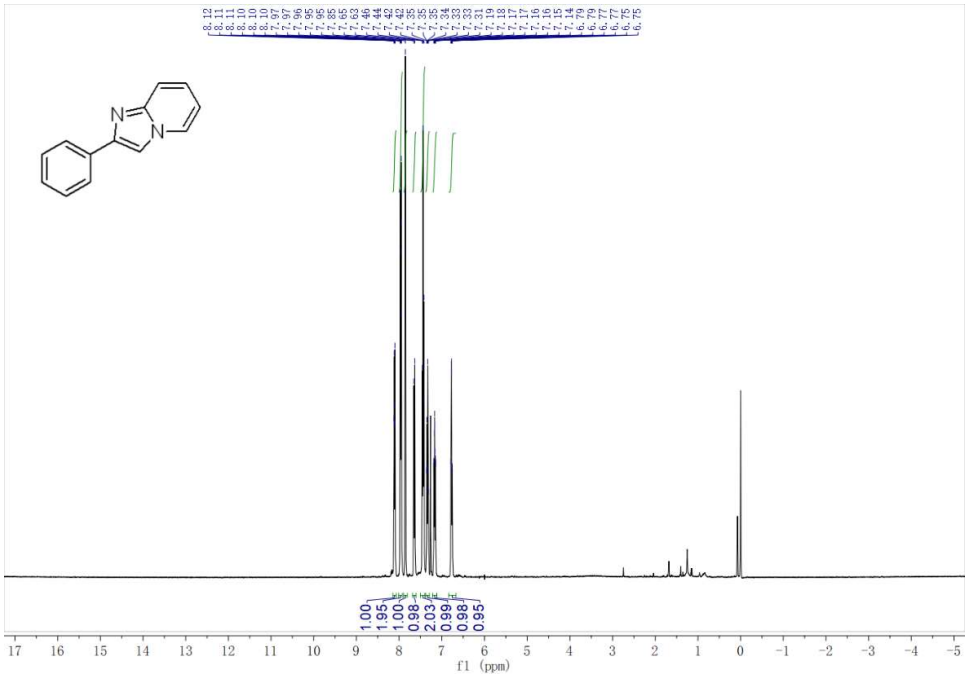
(B) Copies of the ^{1}H-NMR and ^{13}C-NMR spectra of all compounds

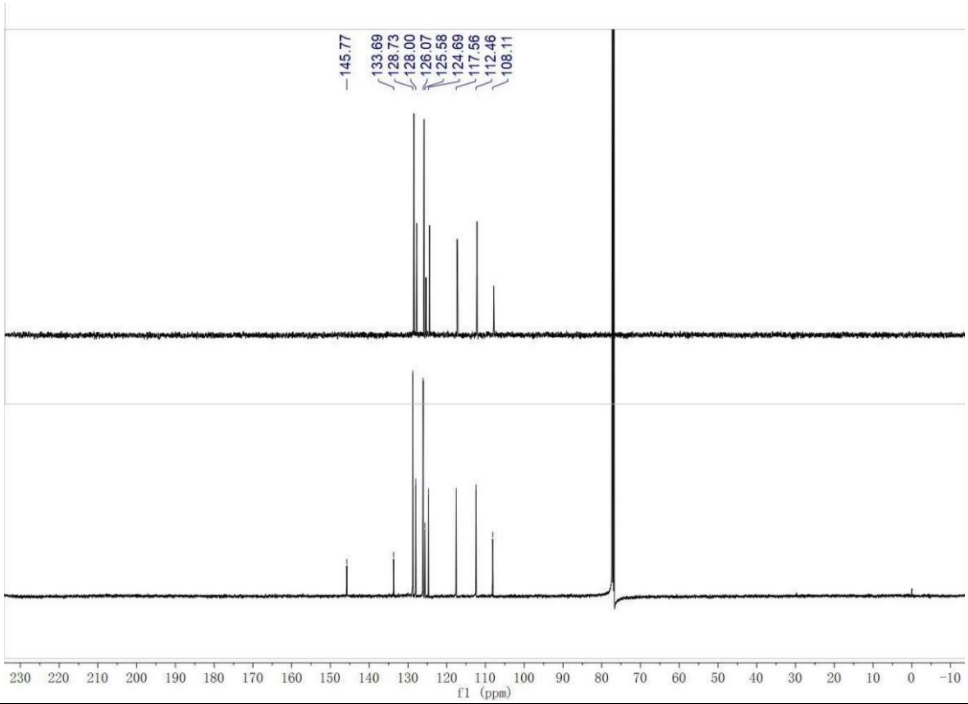
2-Bromo-1-phenylethan-1-one (1aa)



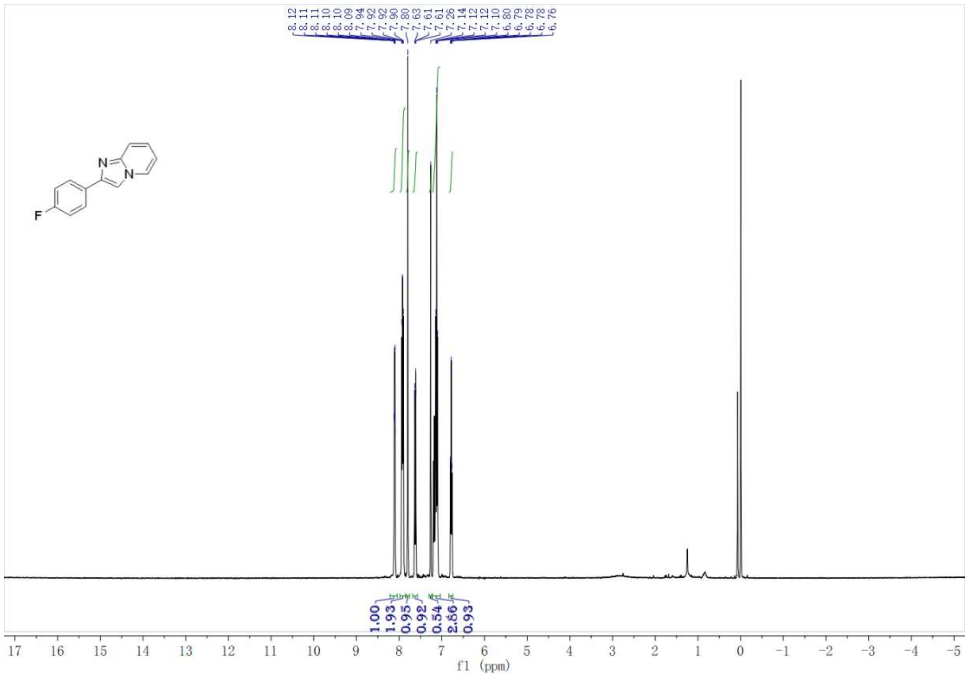


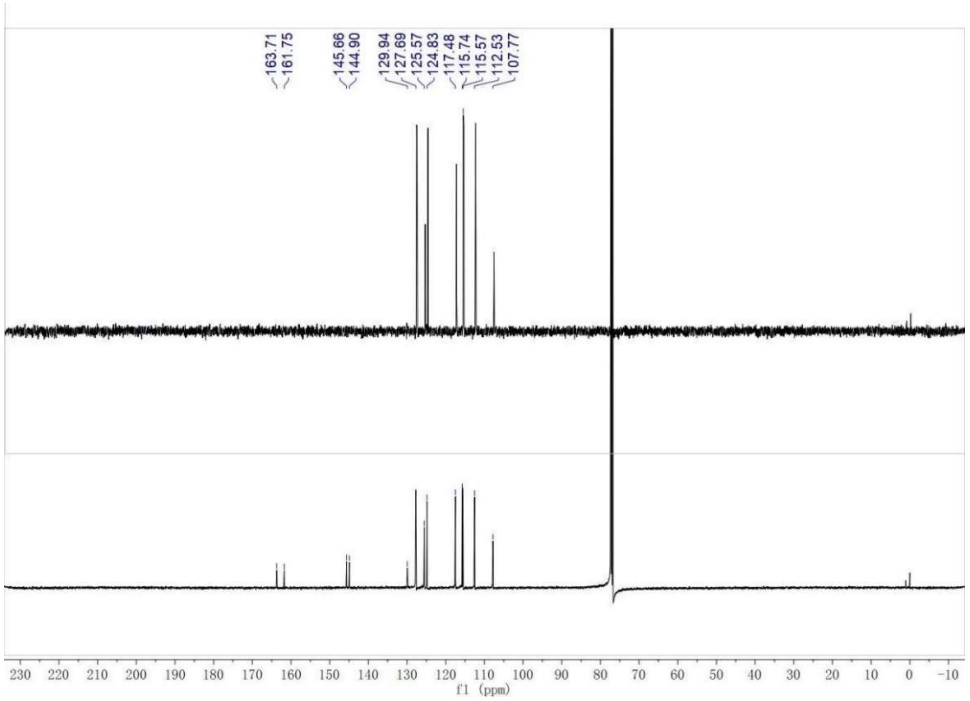
2-Phenylimidazo[1,2-a]pyridine (3a)



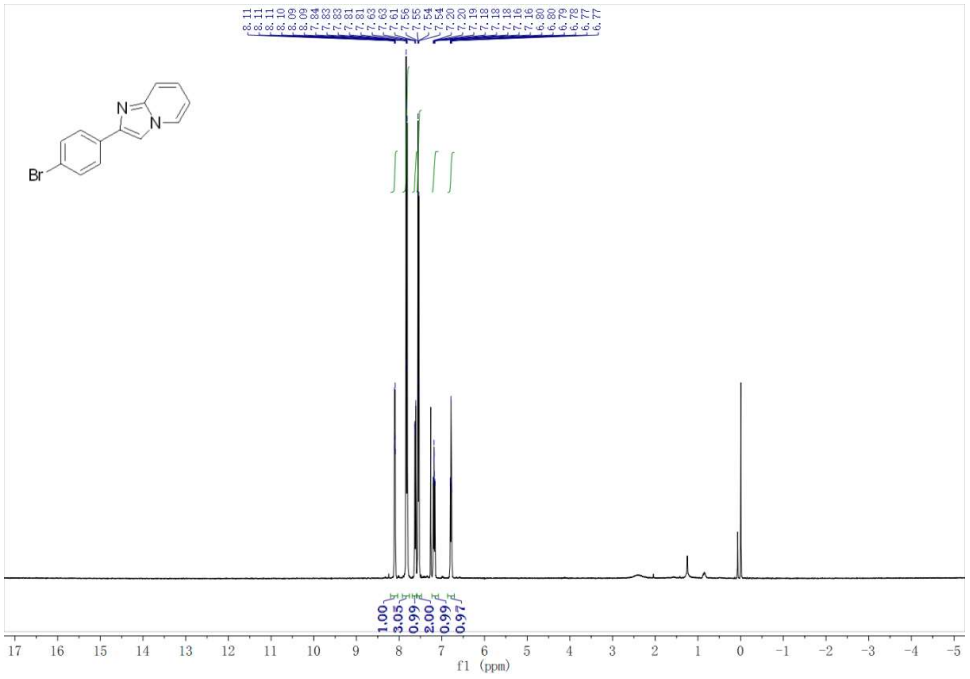


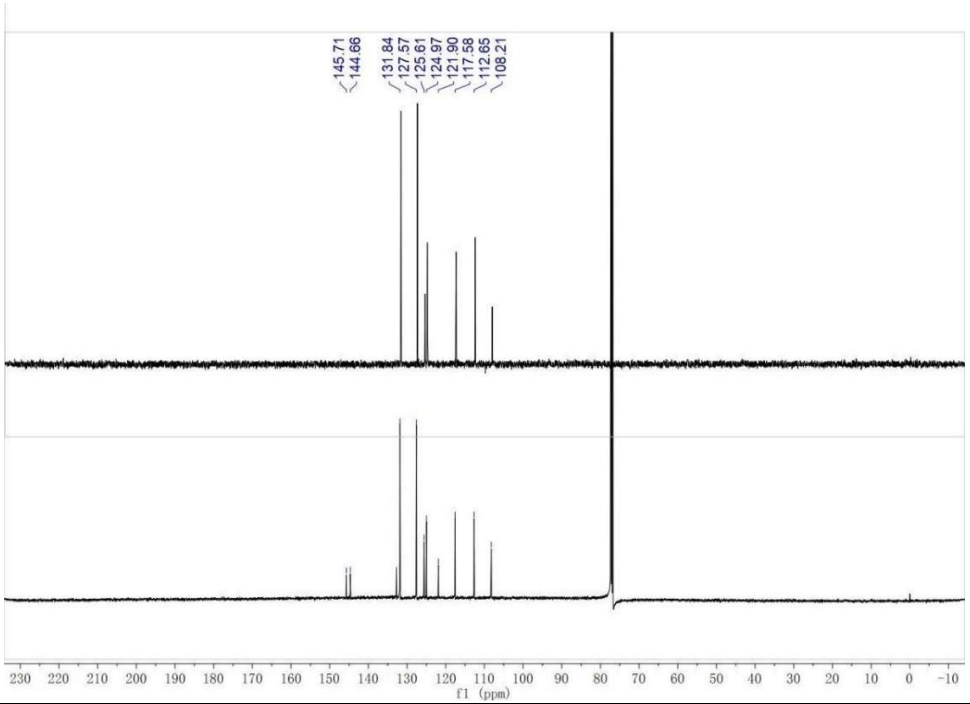
2-(4-Fluorophenyl)imidazo[1,2-a]pyridine (3b)



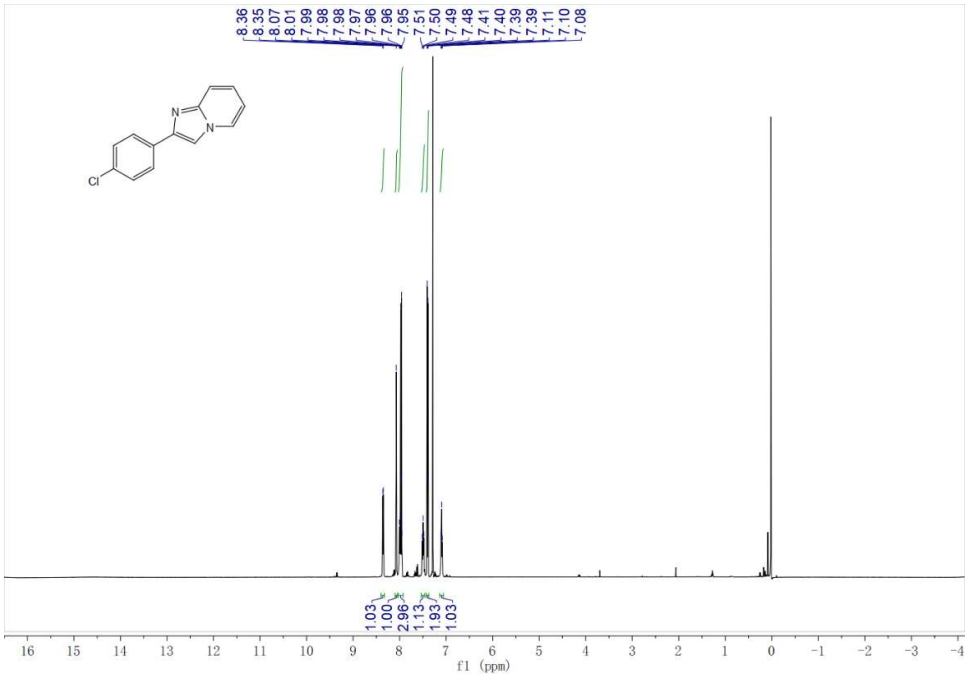


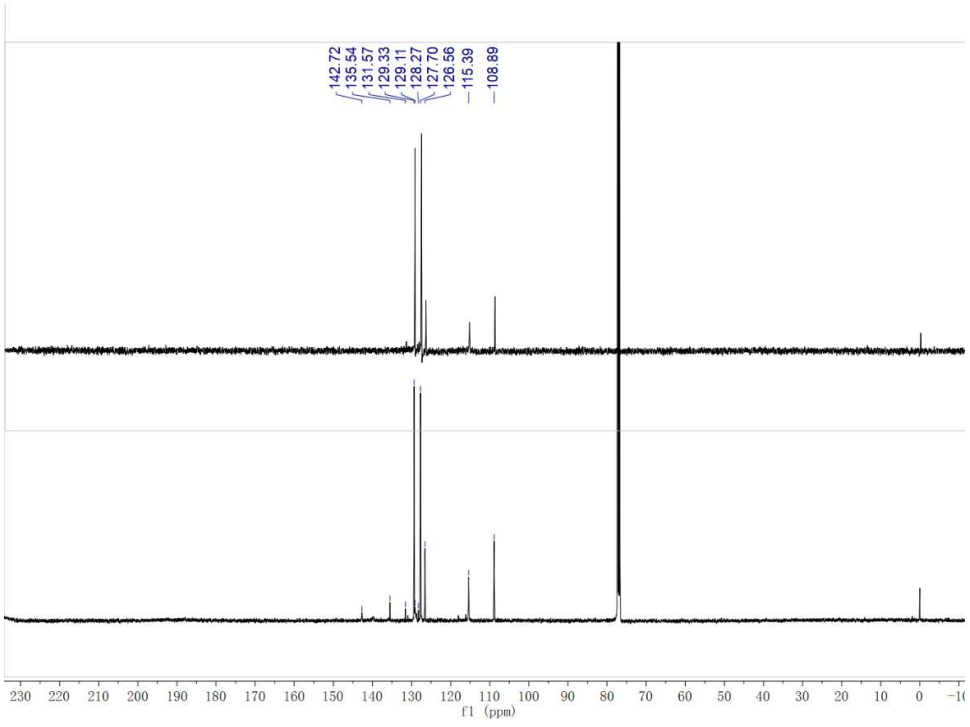
2-(4-Bromophenyl)imidazo[1,2-a]pyridine (3c)



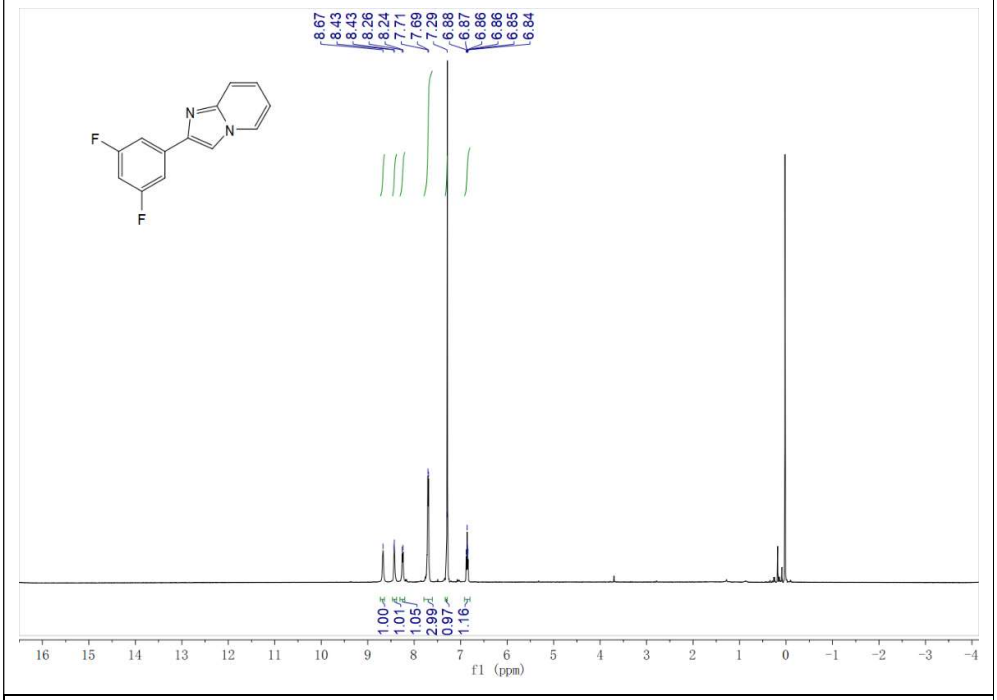


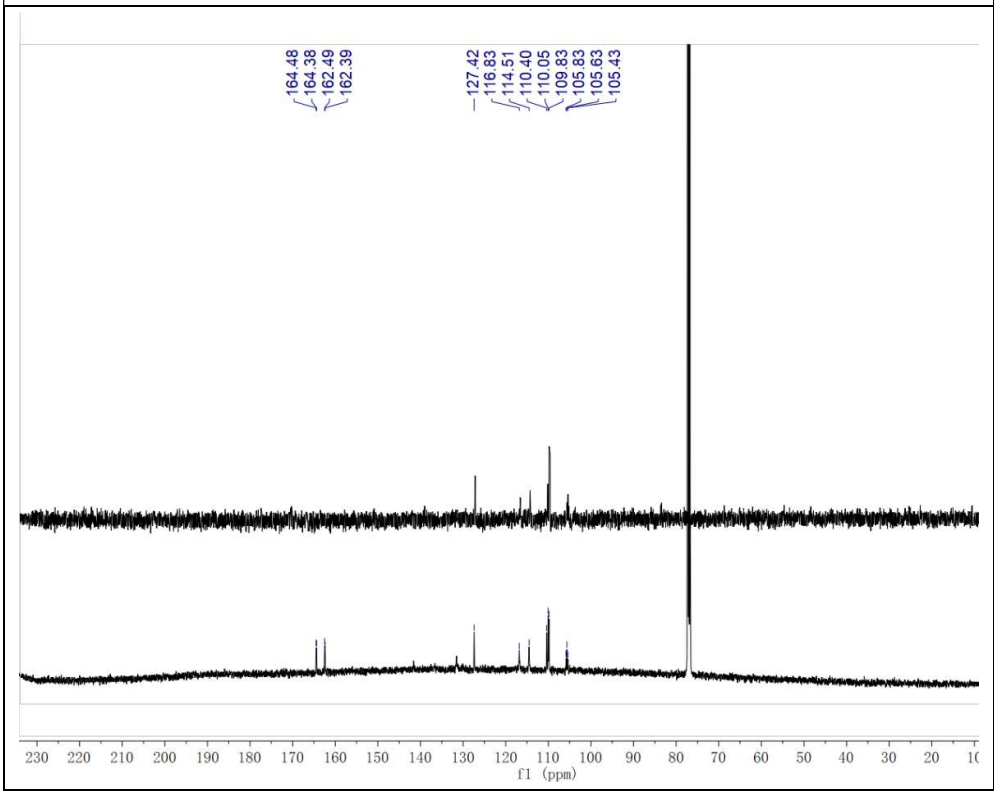
2-(4-Chlorophenyl)imidazo[1,2-a]pyridine (3d)



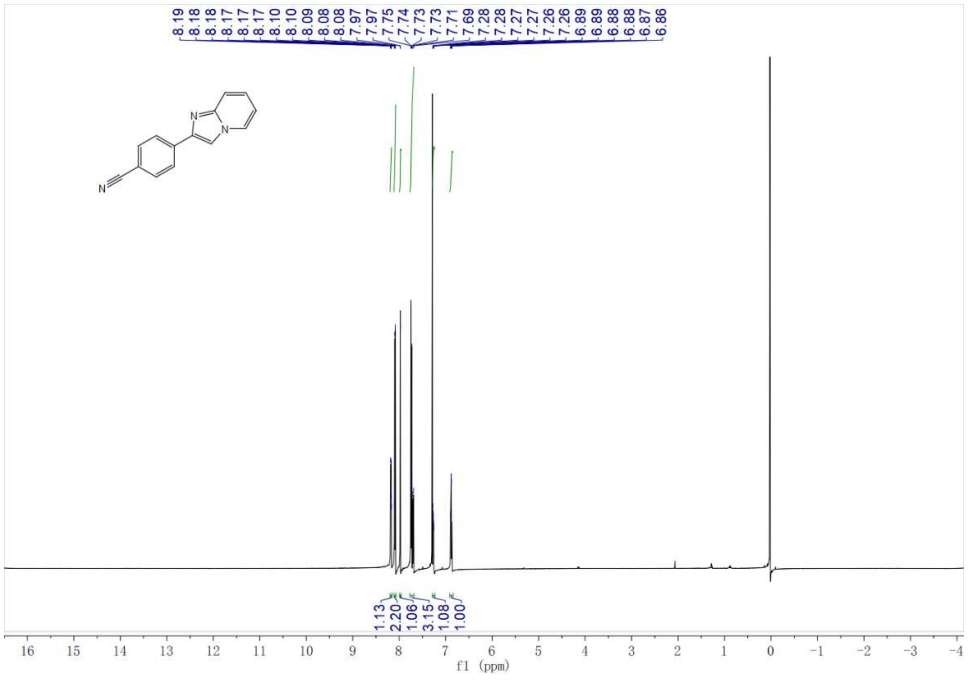


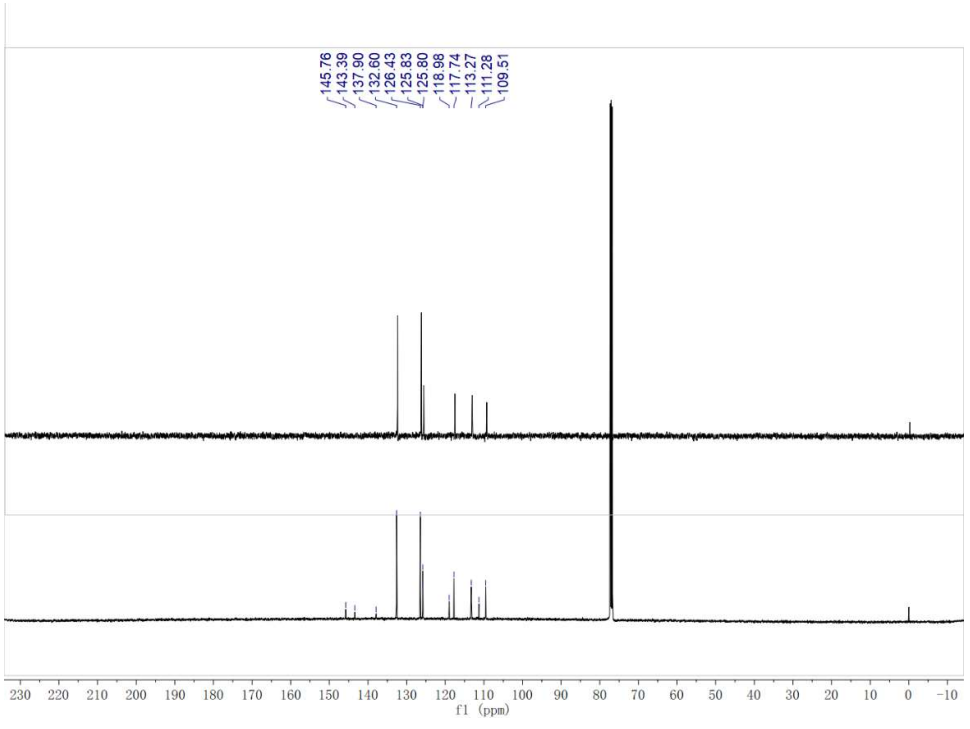
2-(3,5-Difluorophenyl)imidazo[1,2-a]pyridine (3e)



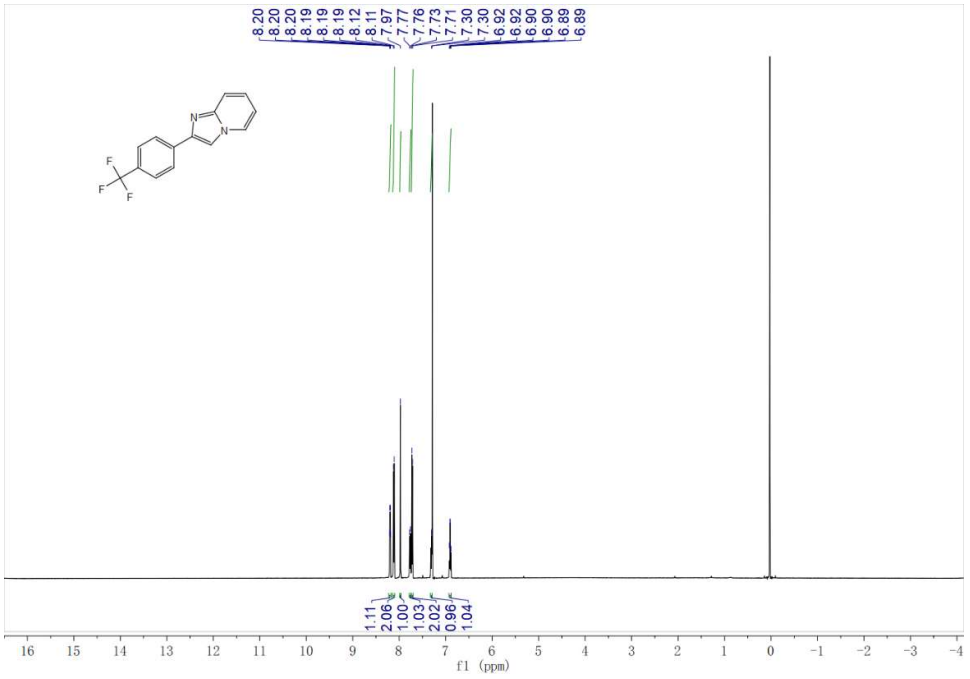


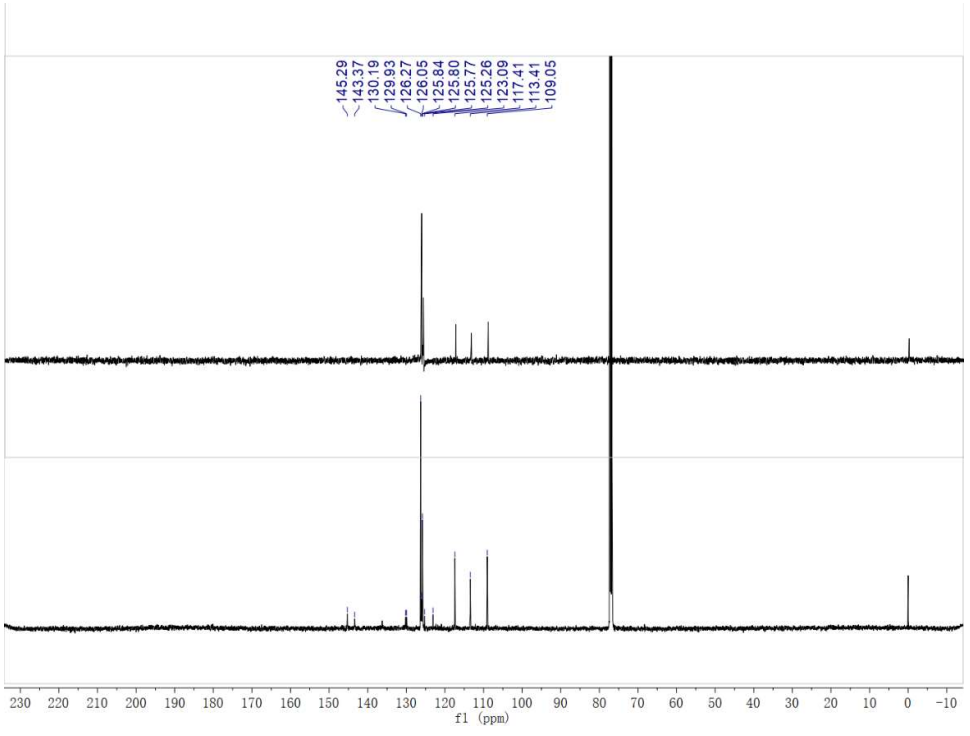
4-(Imidazo[1,2-a]pyridin-2-yl)benzonitrile (3f)



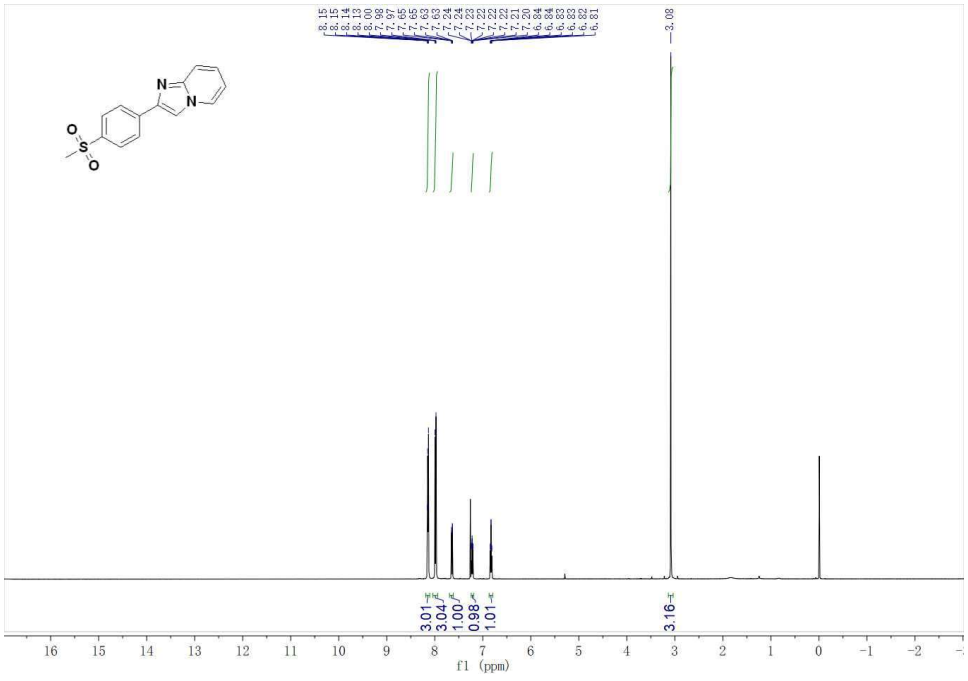


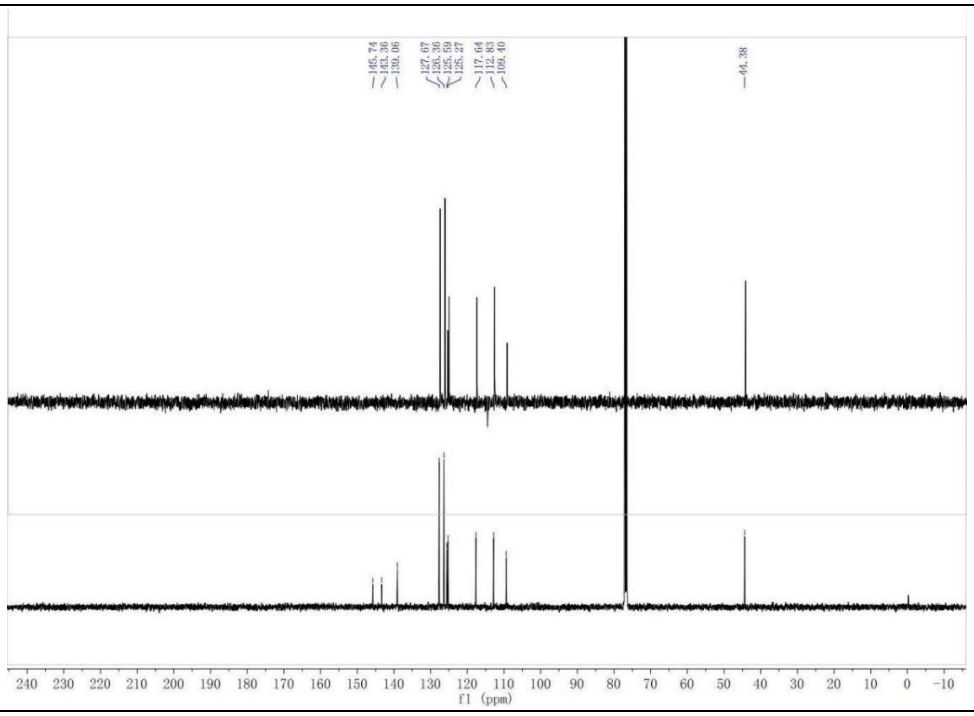
2-(4-(Trifluoromethyl)phenyl)imidazo[1,2-a]pyridine (3g)



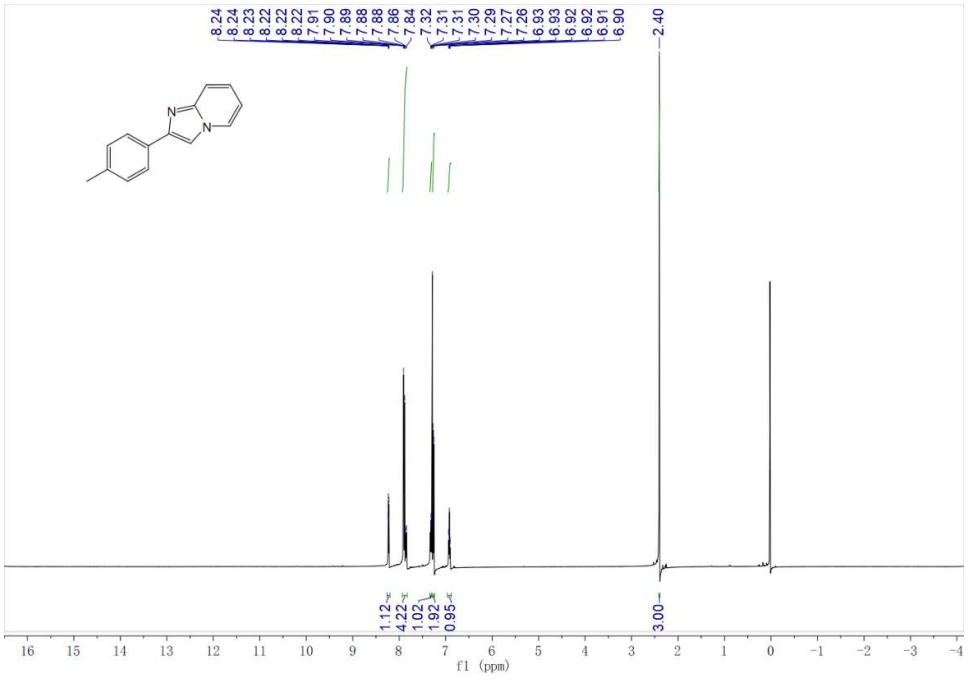


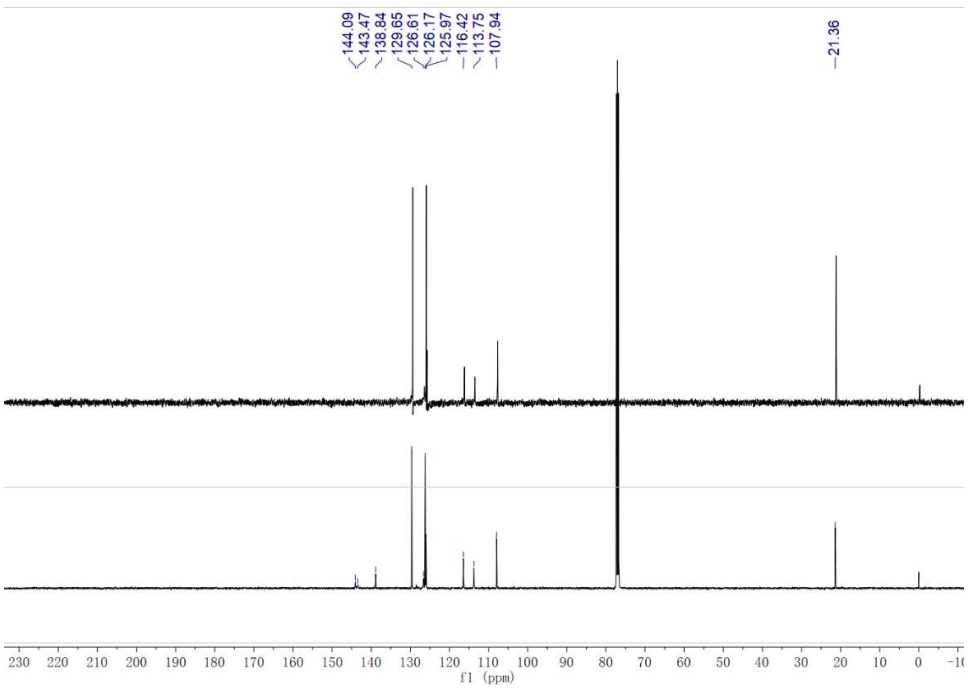
2-(4-(Methylsulfonyl)phenyl)imidazo[1,2-a]pyridine (3h)



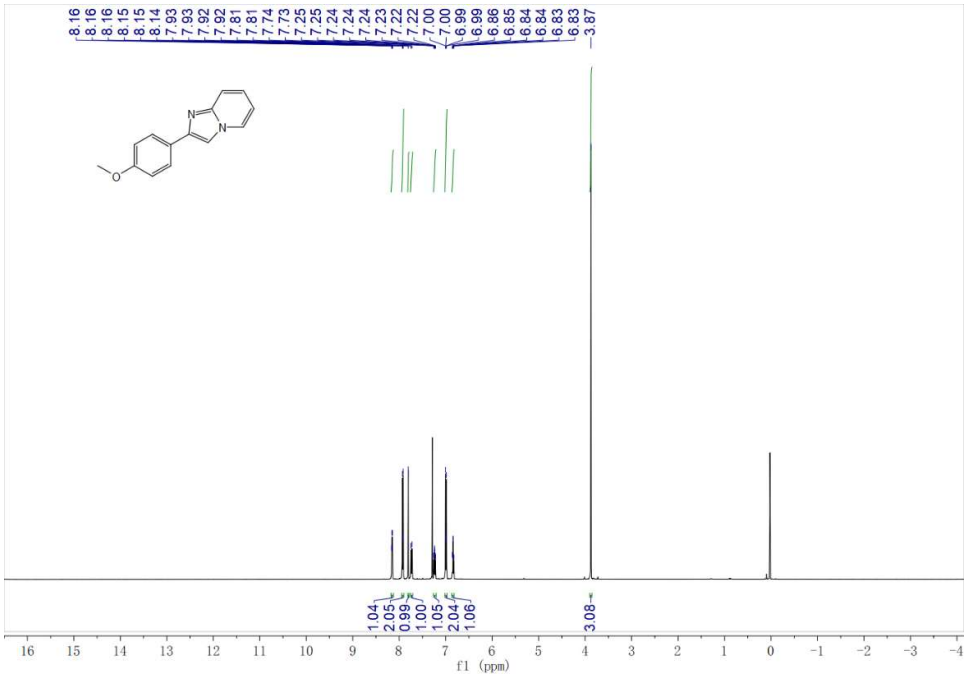


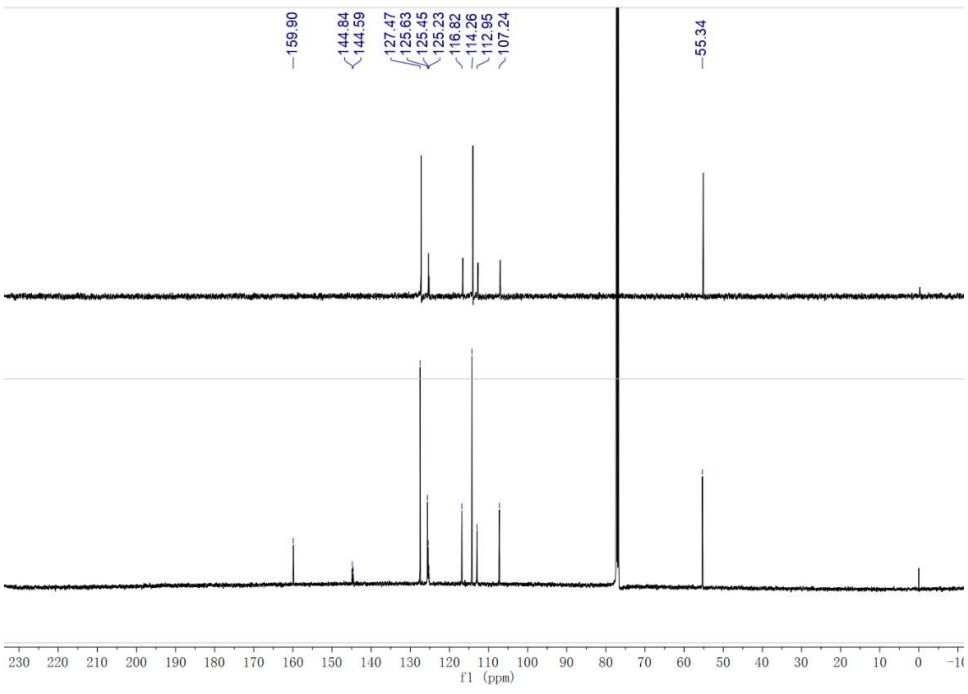
2-(*p*-Tolyl)imidazo[1,2-a]pyridine (3i)



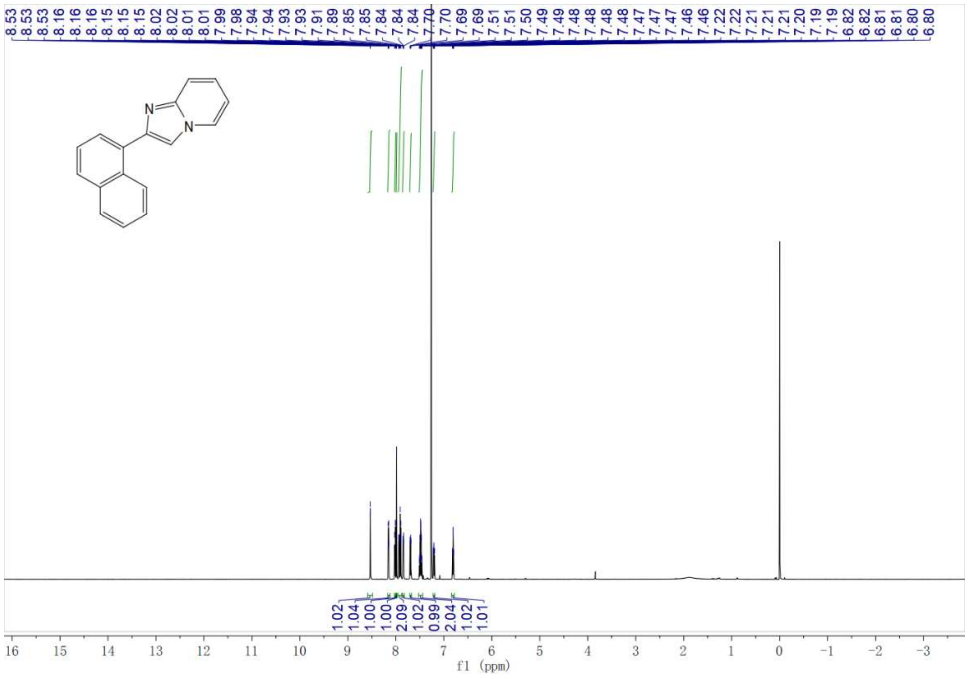


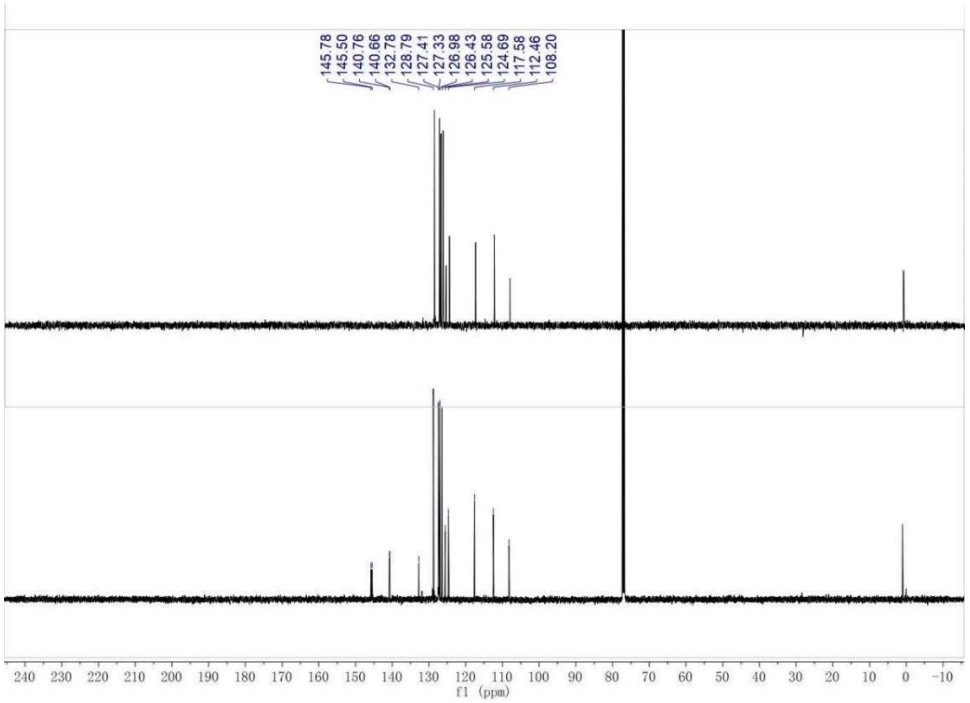
2-(4-Methoxyphenyl)imidazo[1,2-a]pyridine (3j)



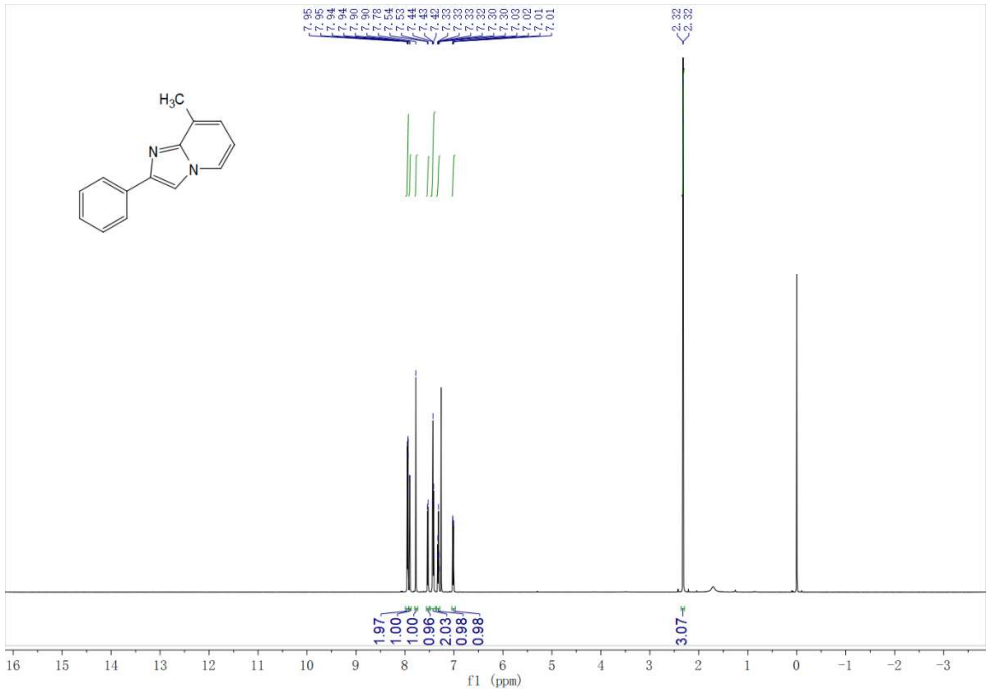


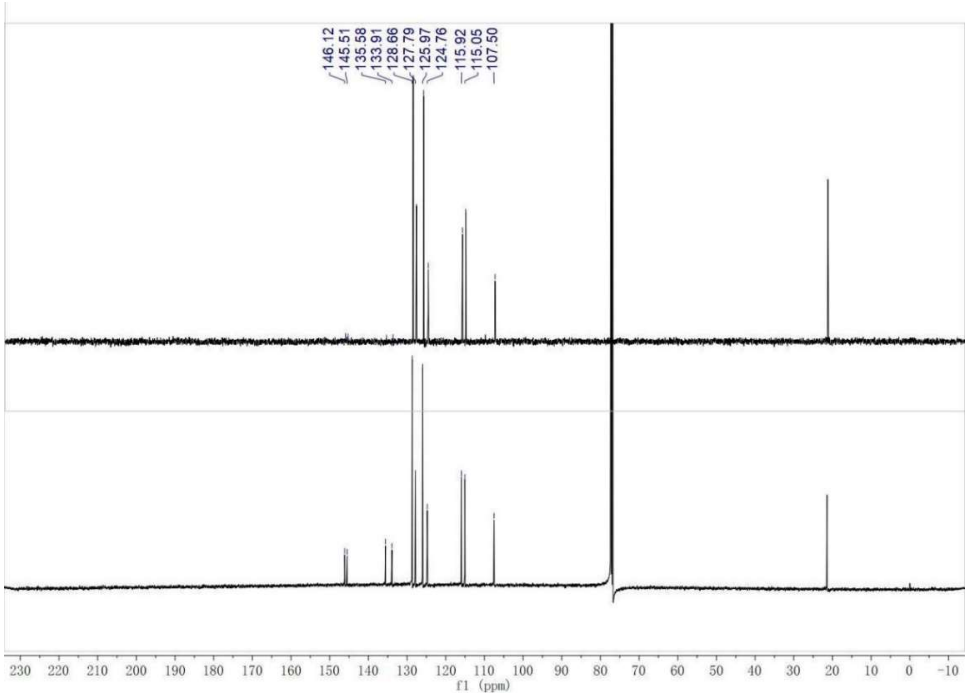
2-(Naphthalen-1-yl)imidazo[1,2-a]pyridine (3k)



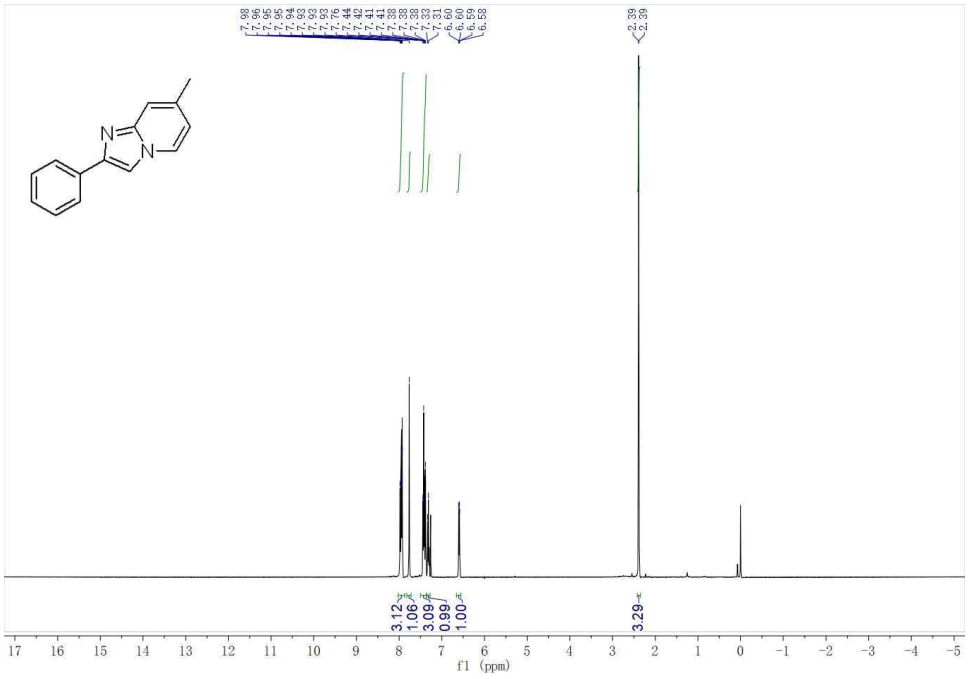


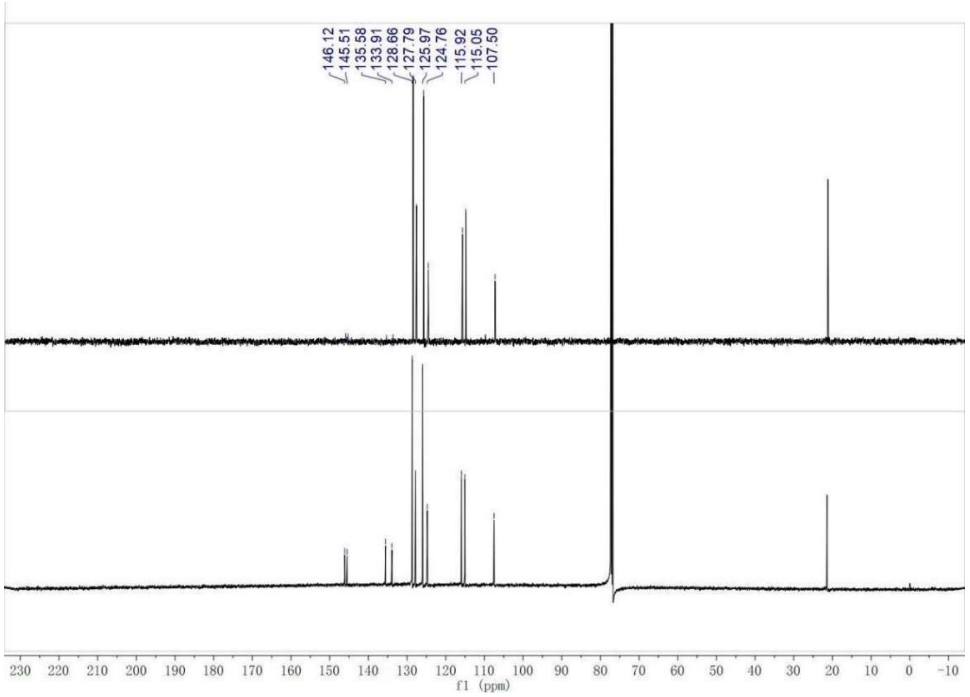
8-Methyl-2-phenylimidazo[1,2-a]pyridine (3l)



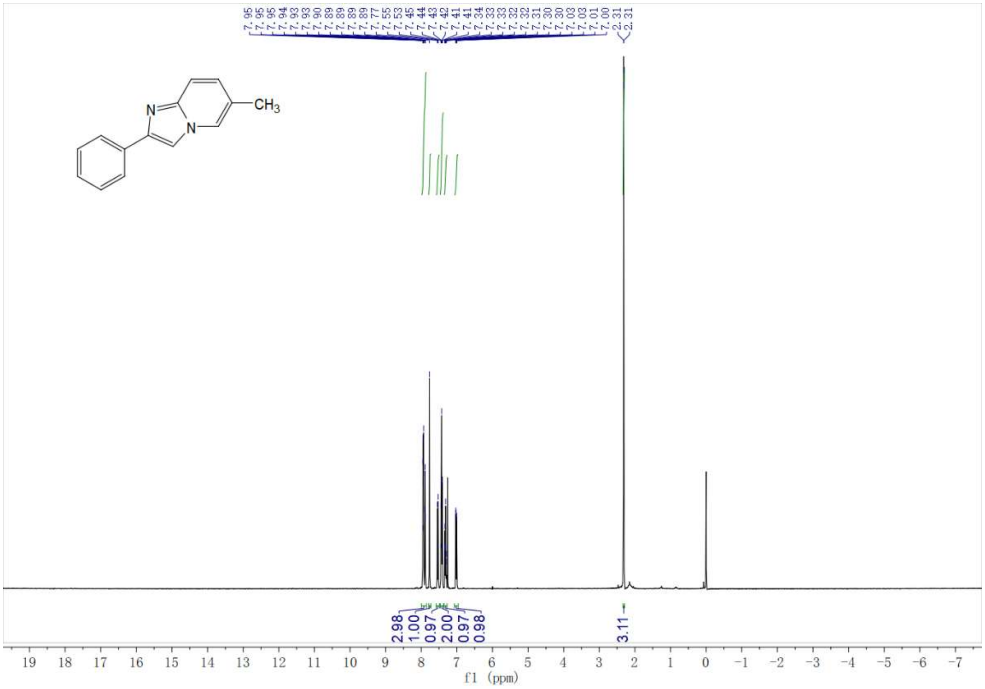


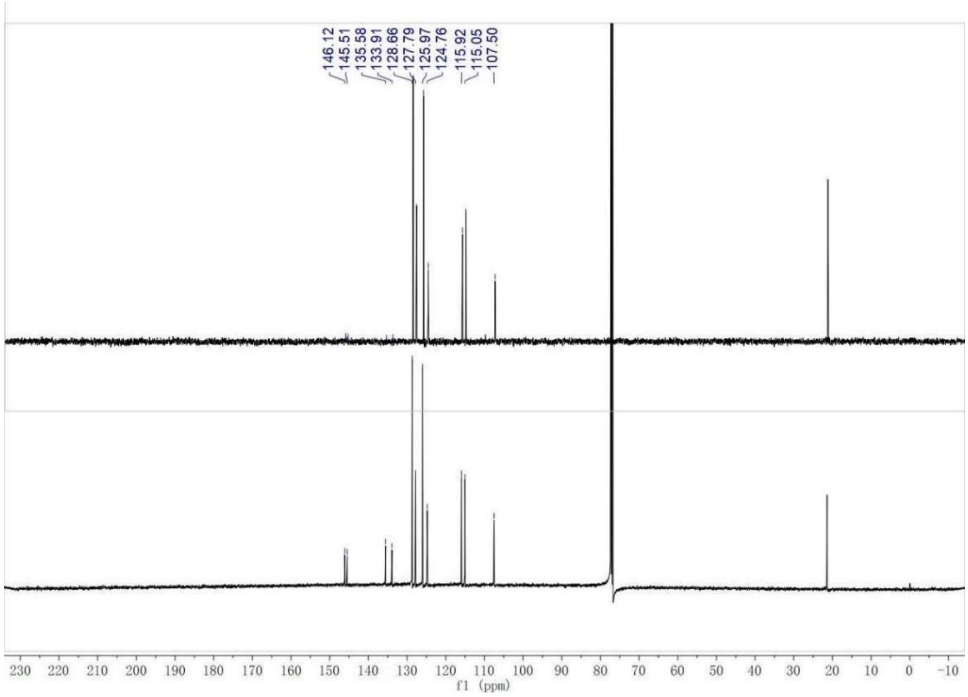
7-Methyl-2-phenylimidazo[1,2-a]pyridine (3m)



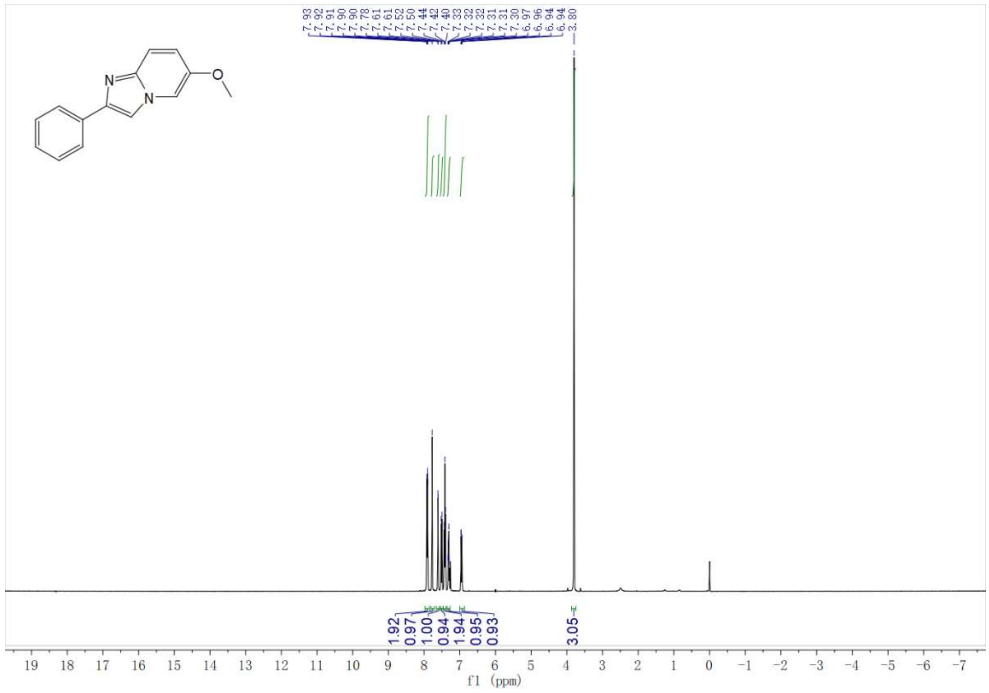


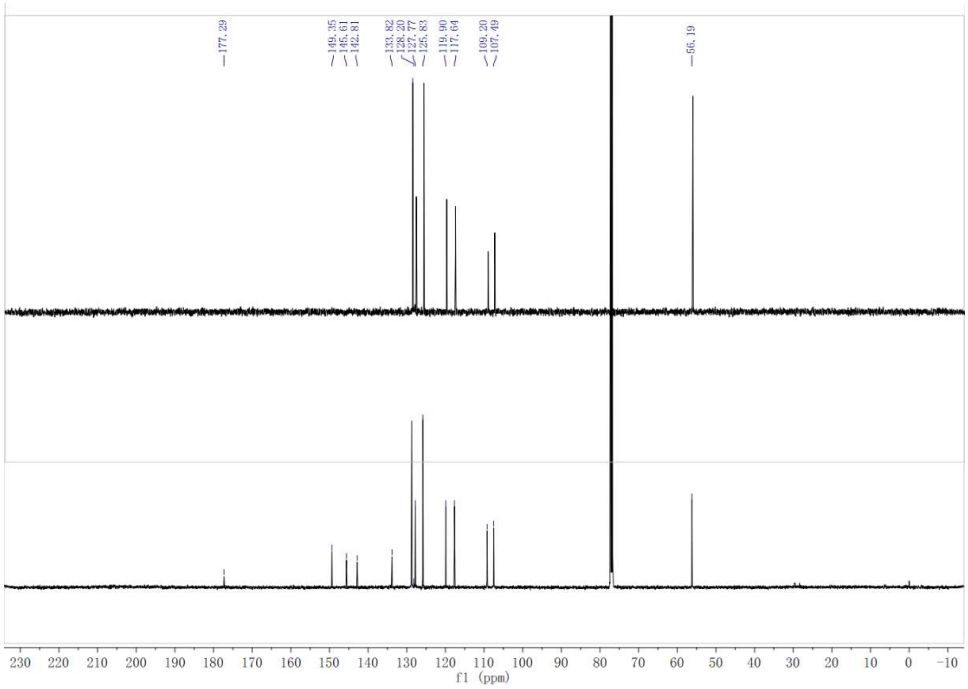
6-Methyl-2-phenylimidazo[1,2-a]pyridine (3n)



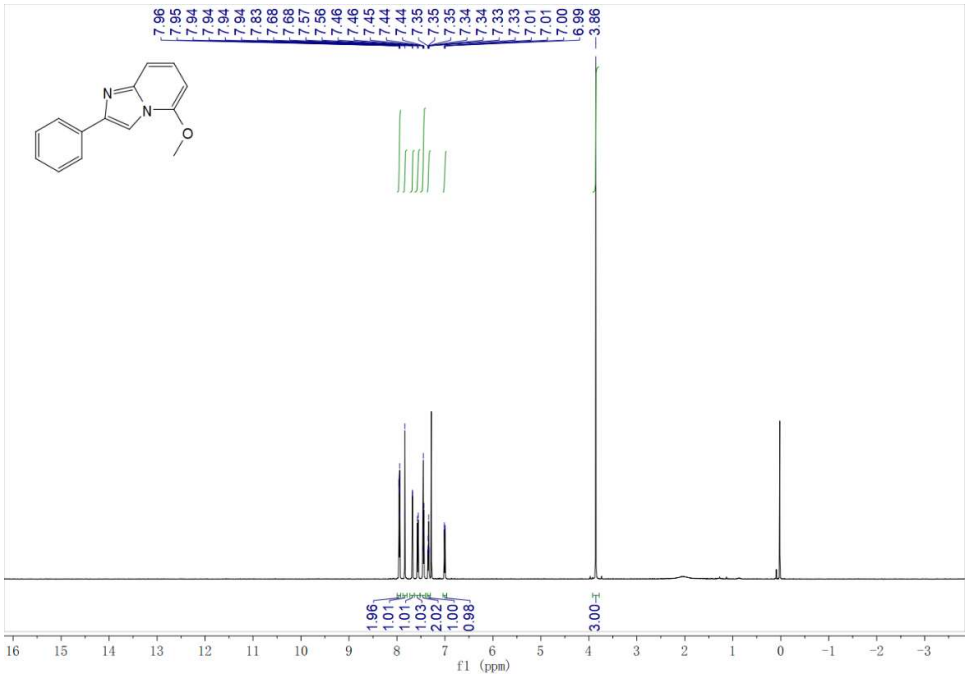


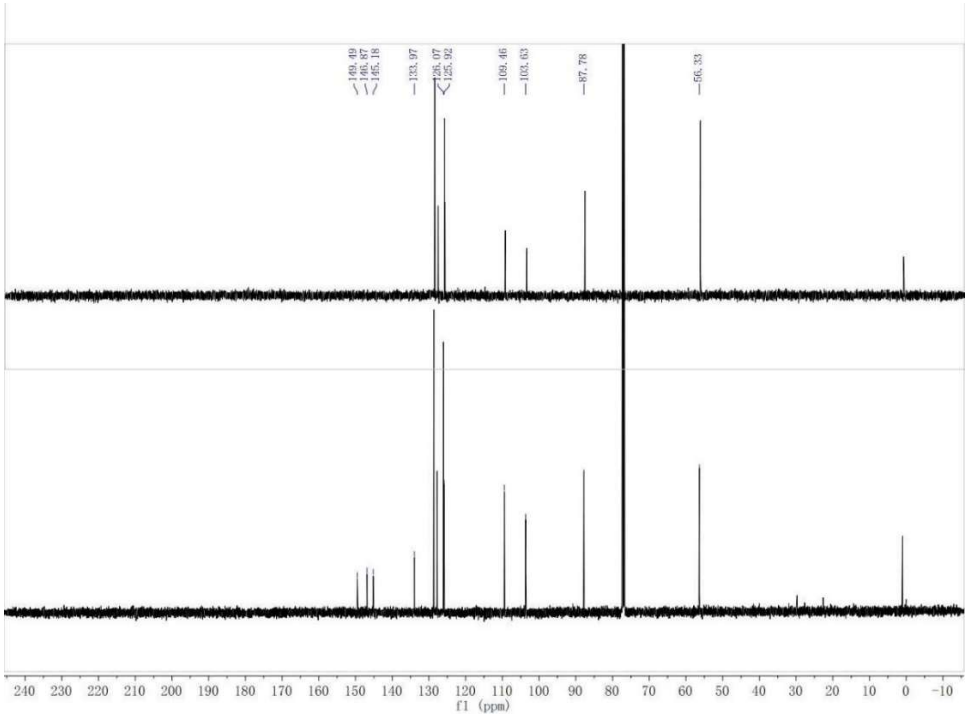
6-Methoxy-2-phenylimidazo[1,2-a]pyridine (3o)



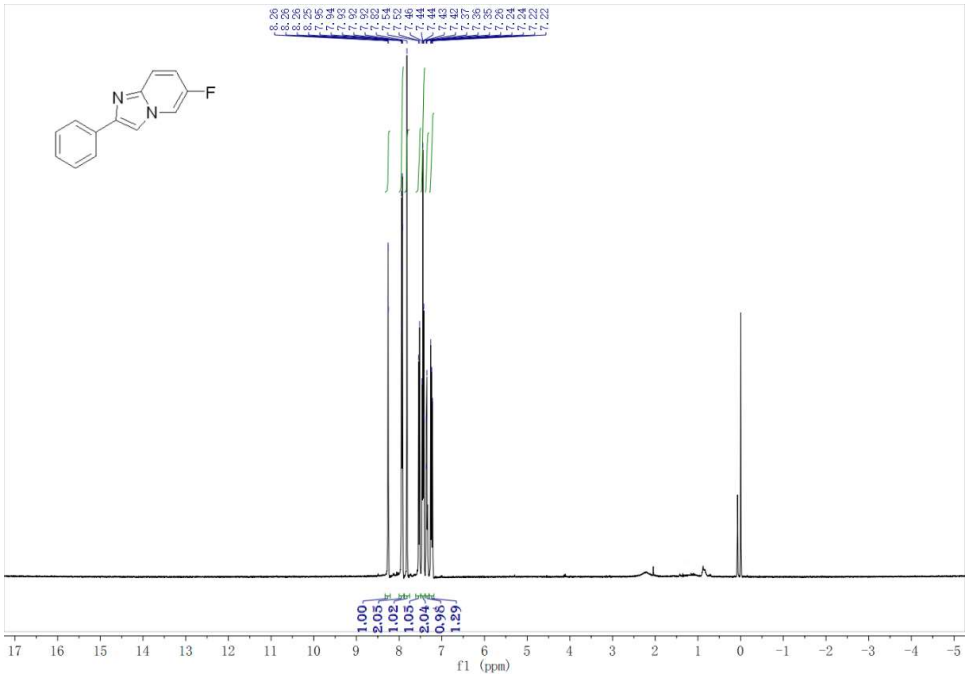


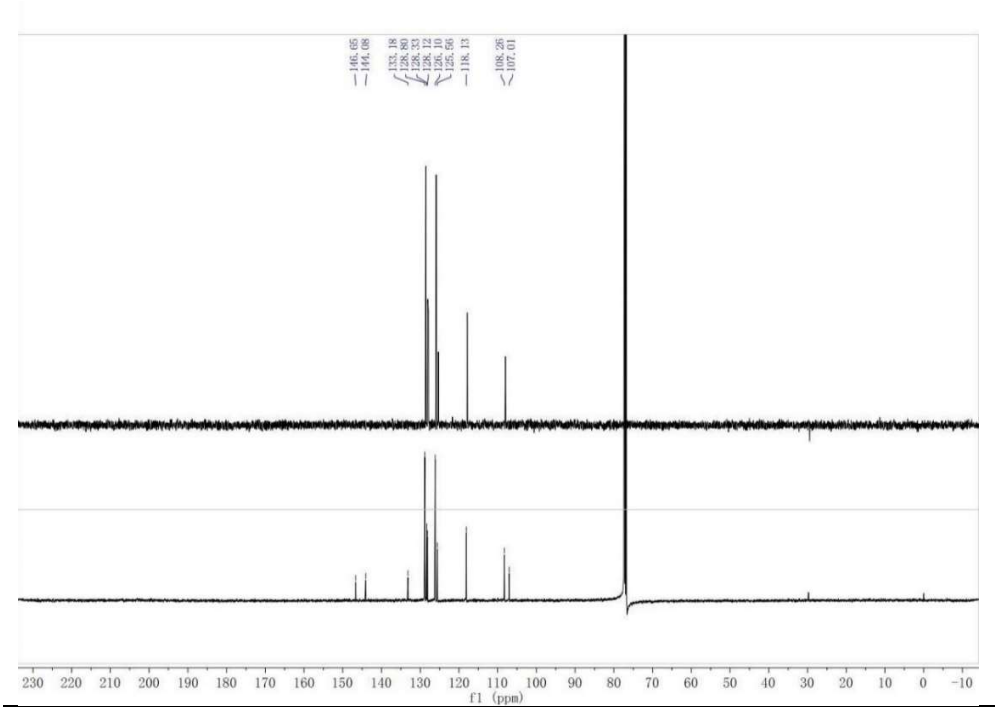
5-Methoxy-2-phenylimidazo[1,2-a]pyridine (3p)



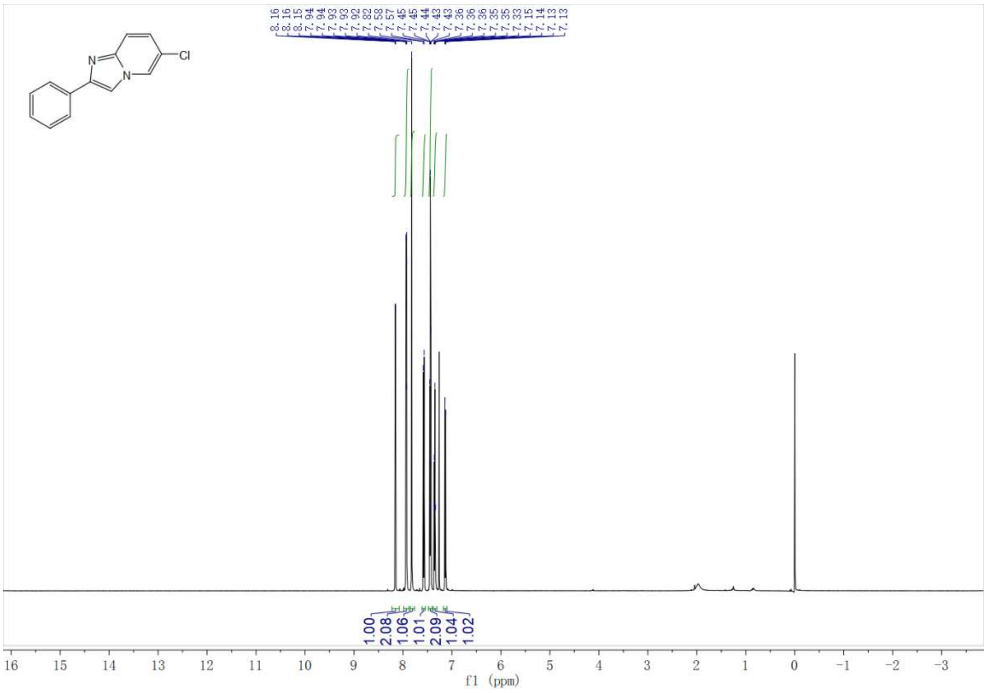


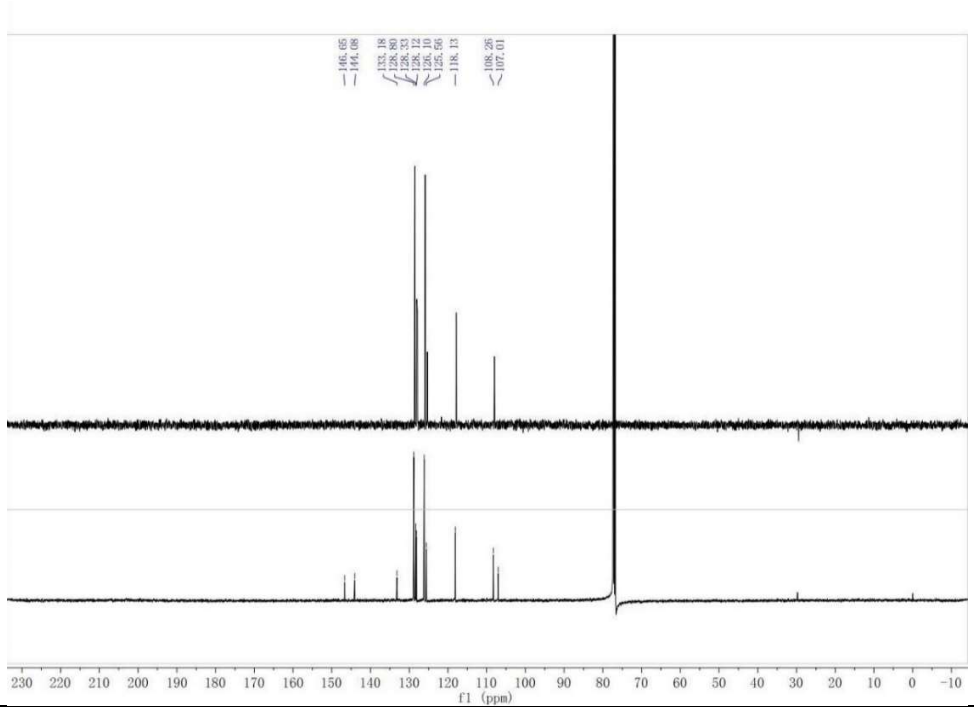
6-Fluoro-2-phenylimidazo[1,2-a]pyridine (3q)



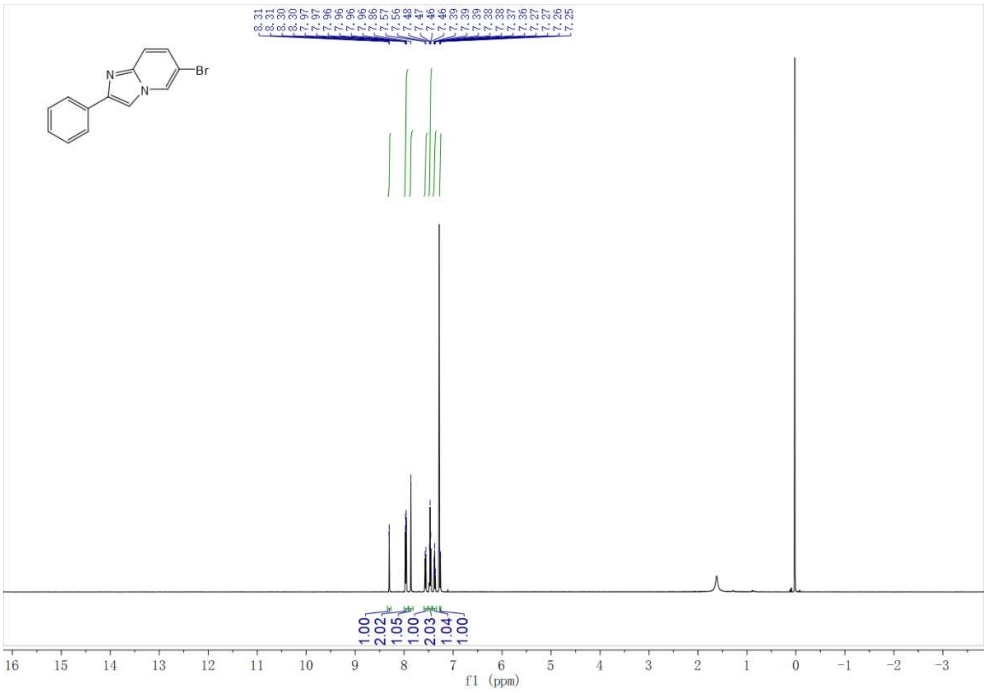


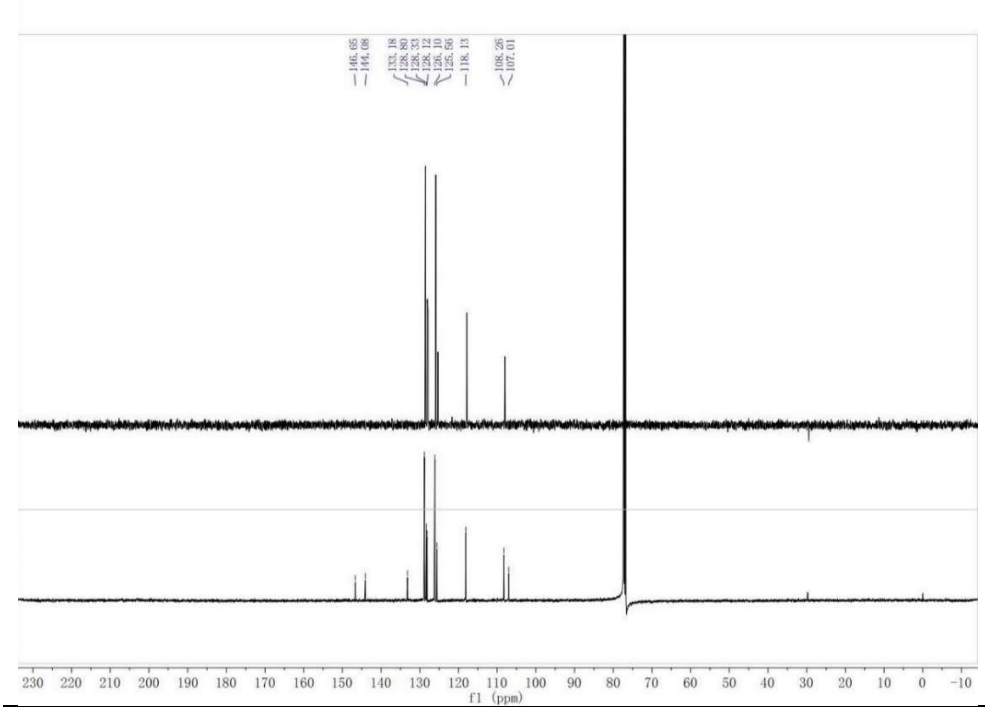
6-Chloro-2-phenylimidazo[1,2-a]pyridine (3r)



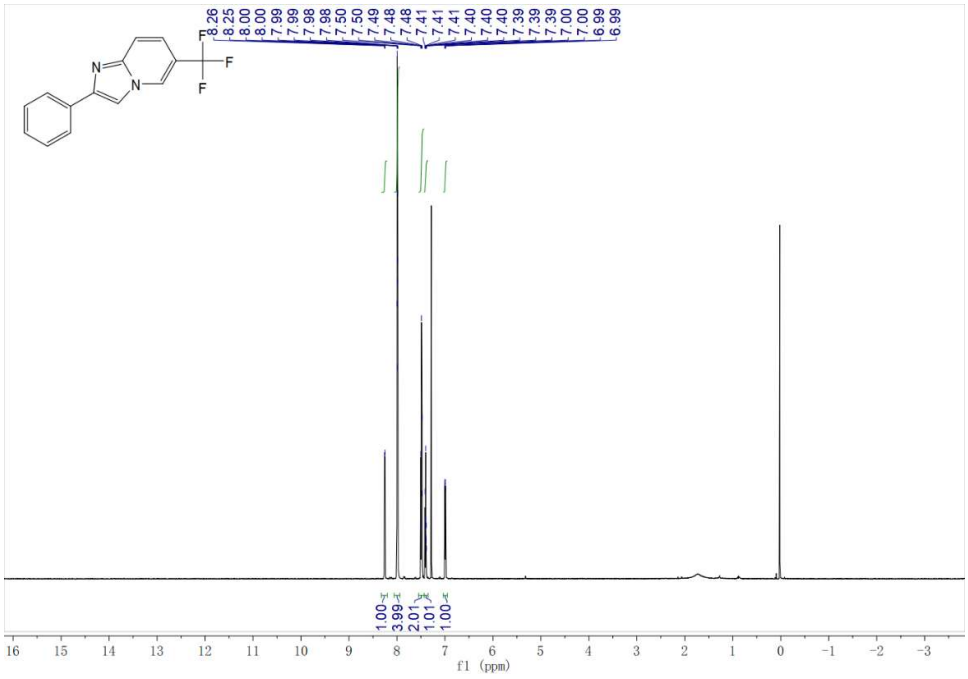


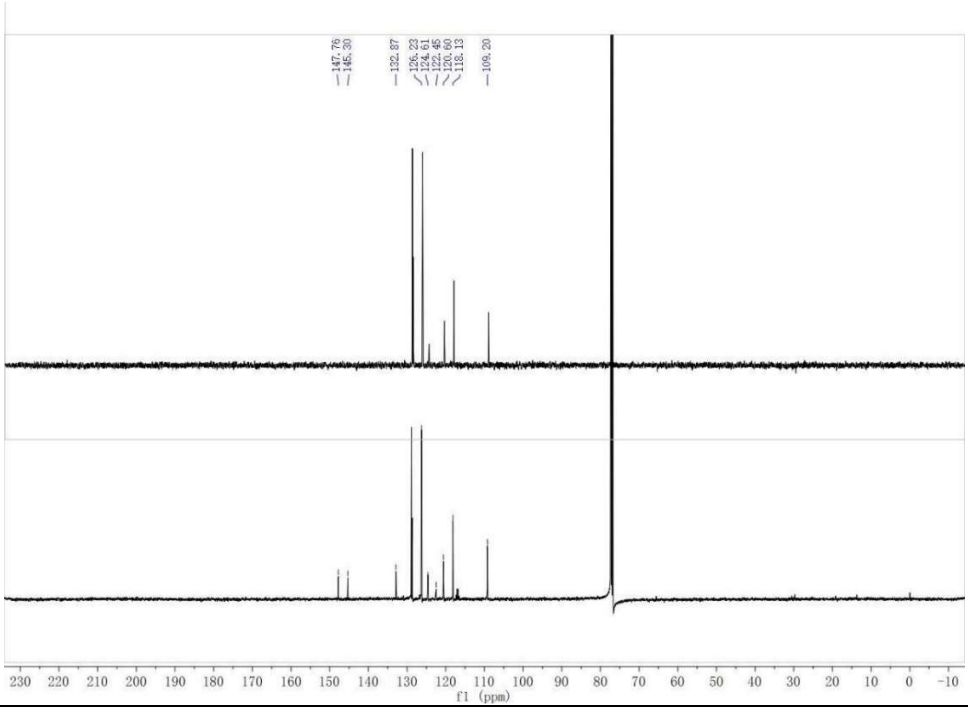
6-Bromo-2-phenylimidazo[1,2-a]pyridine (3s)



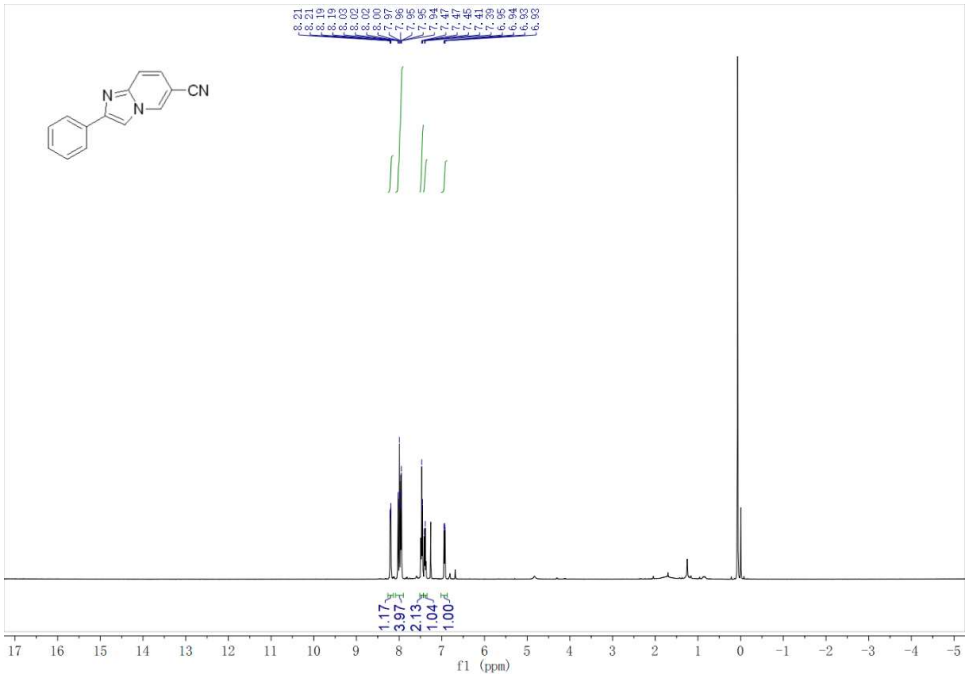


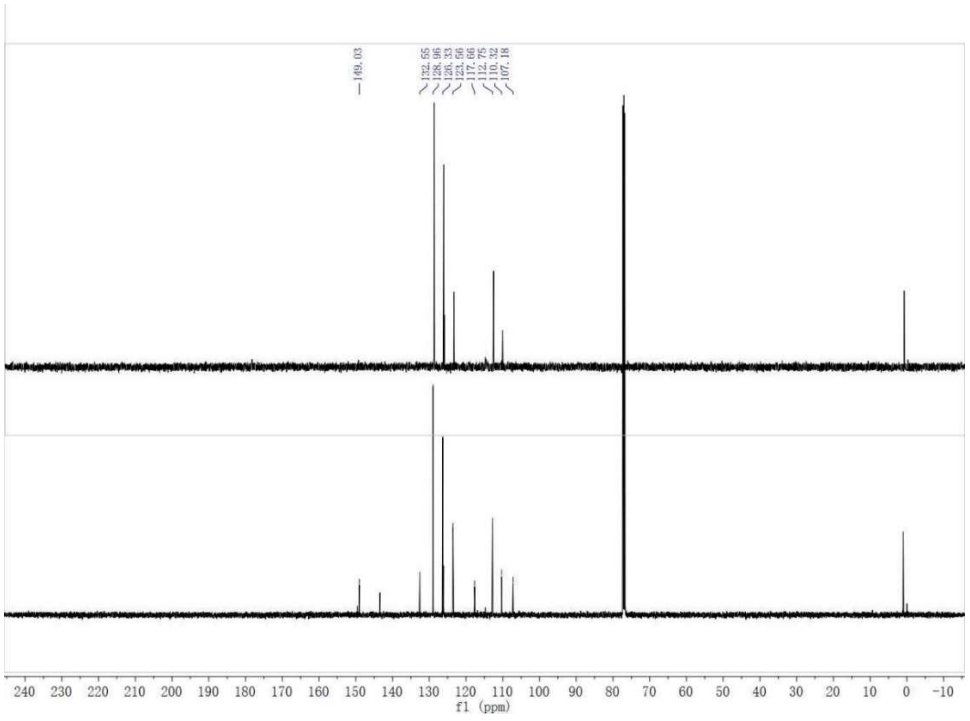
2-Phenyl-6-(trifluoromethyl)imidazo[1,2-a]pyridine (3t)



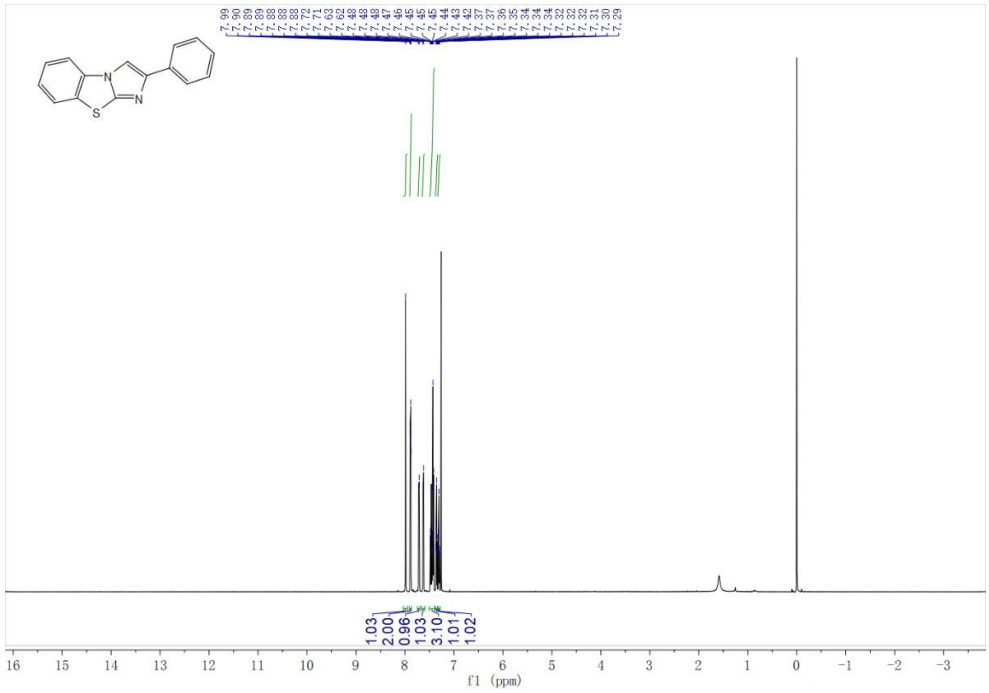


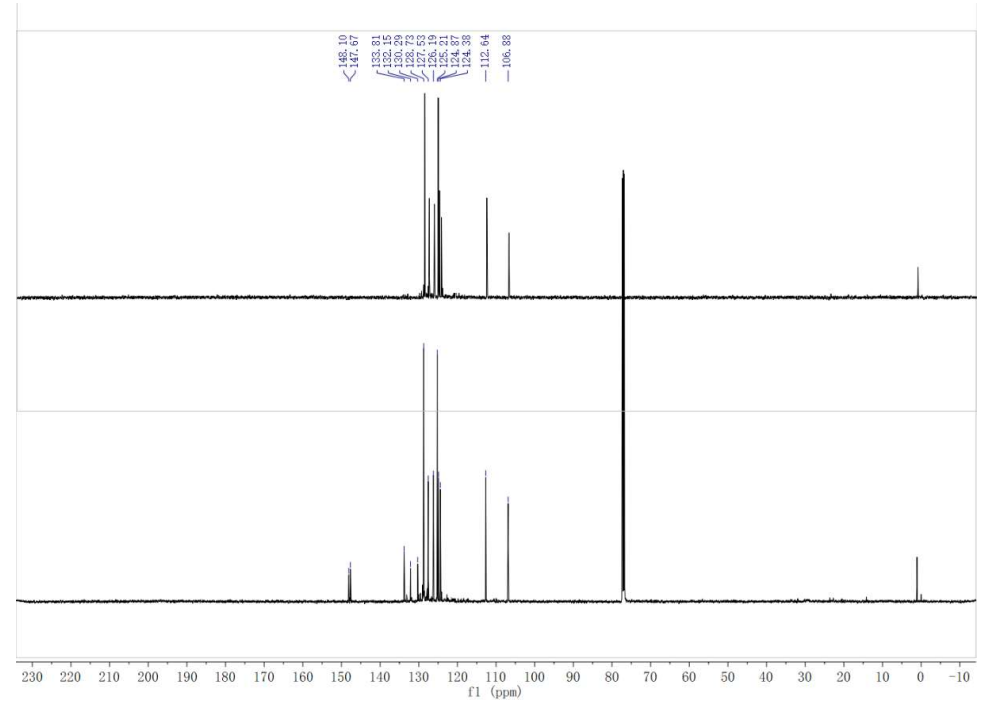
2-Phenylimidazo[1,2-a]pyridine-6-carbonitrile (3u)



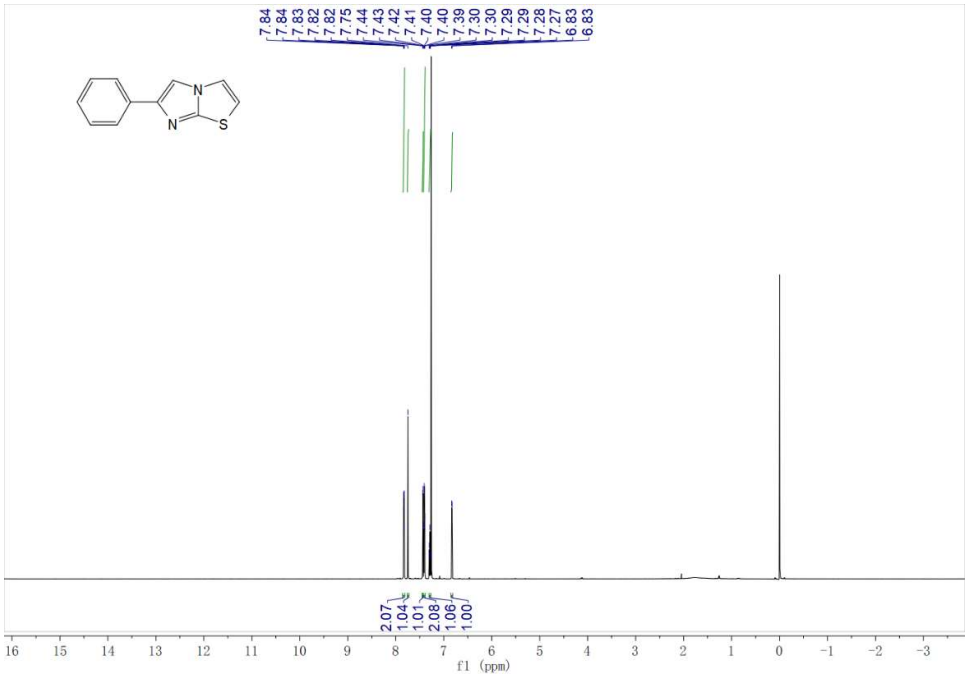


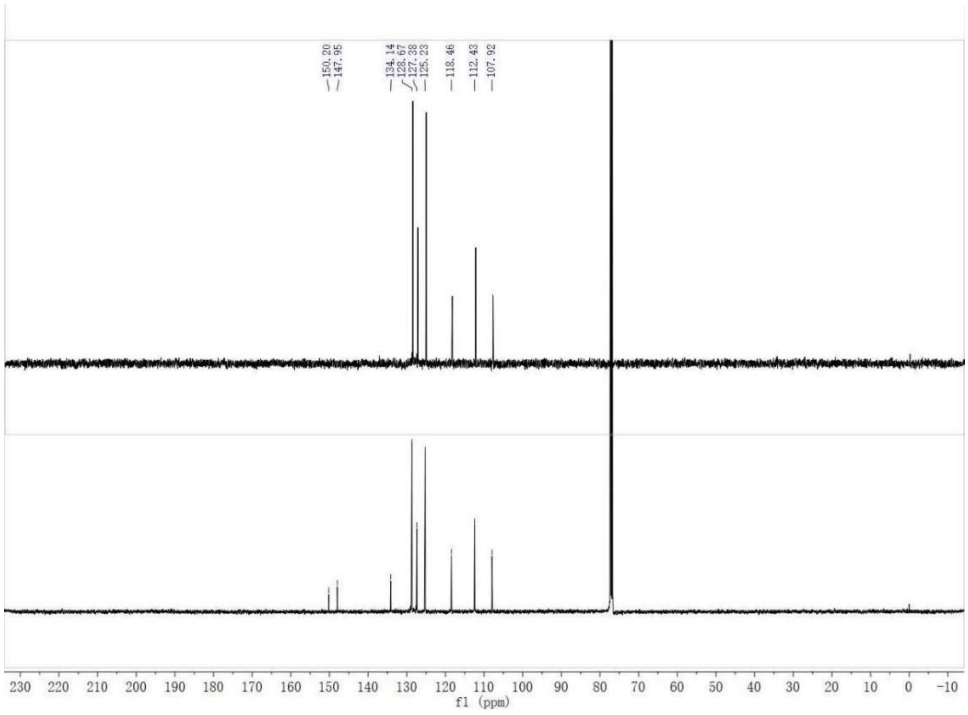
2-Phenylbenzo[d]imidazo[2,1-b]thiazole (5a)



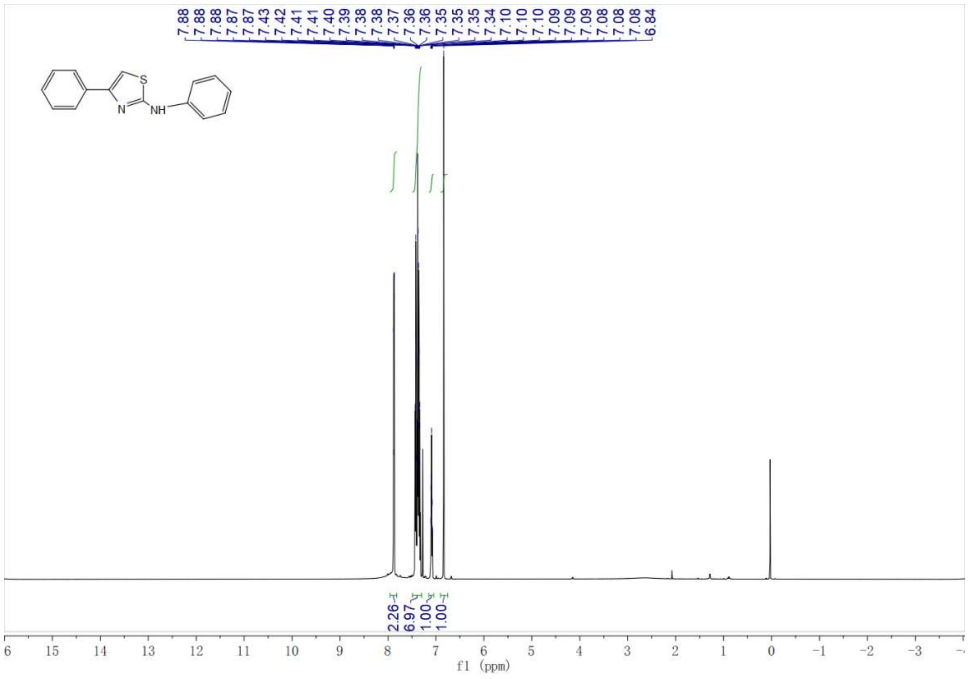


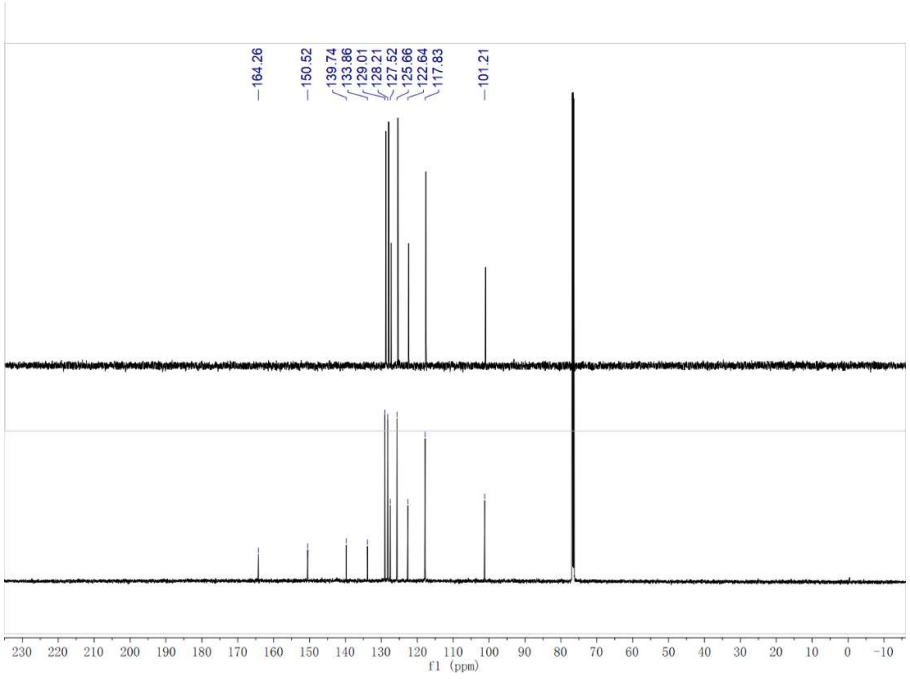
6-Phenylimidazo[2,1-b]thiazole (5b)



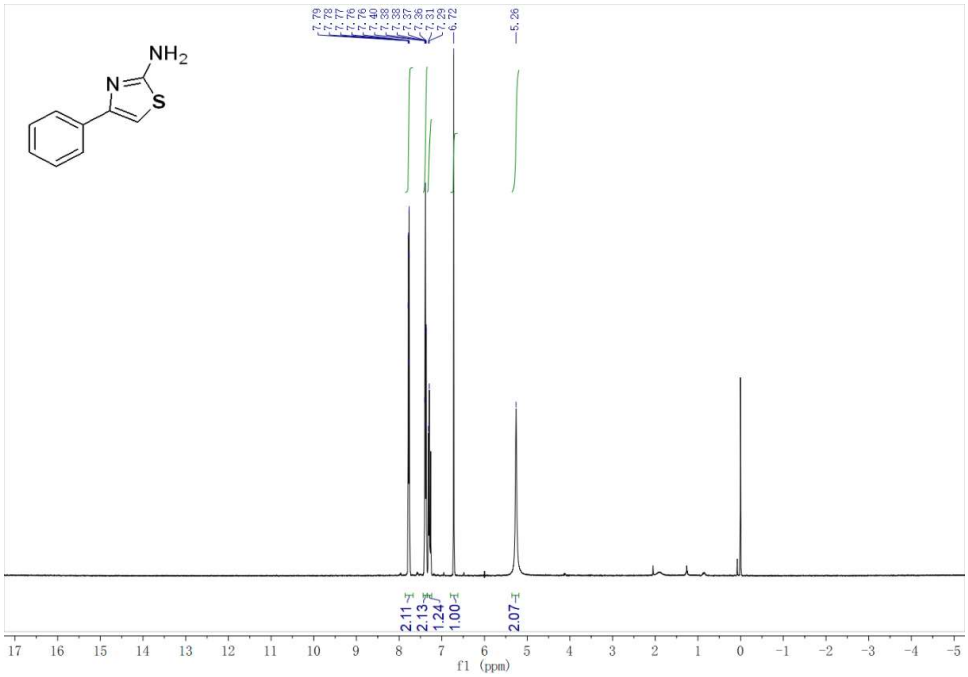


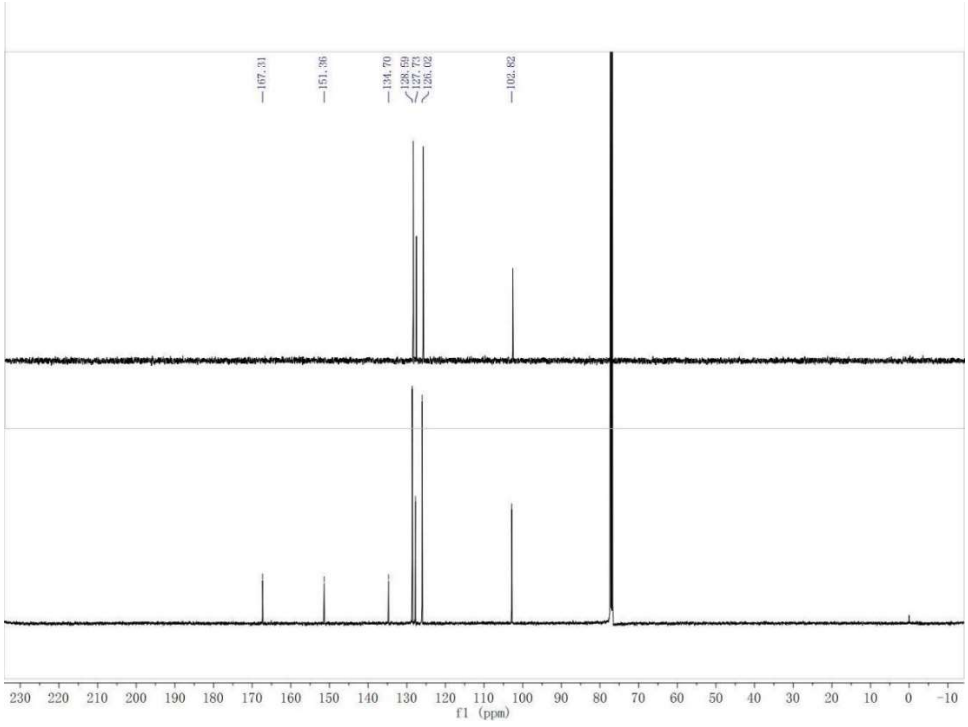
N,4-Diphenylthiazol-2-amine (5c)



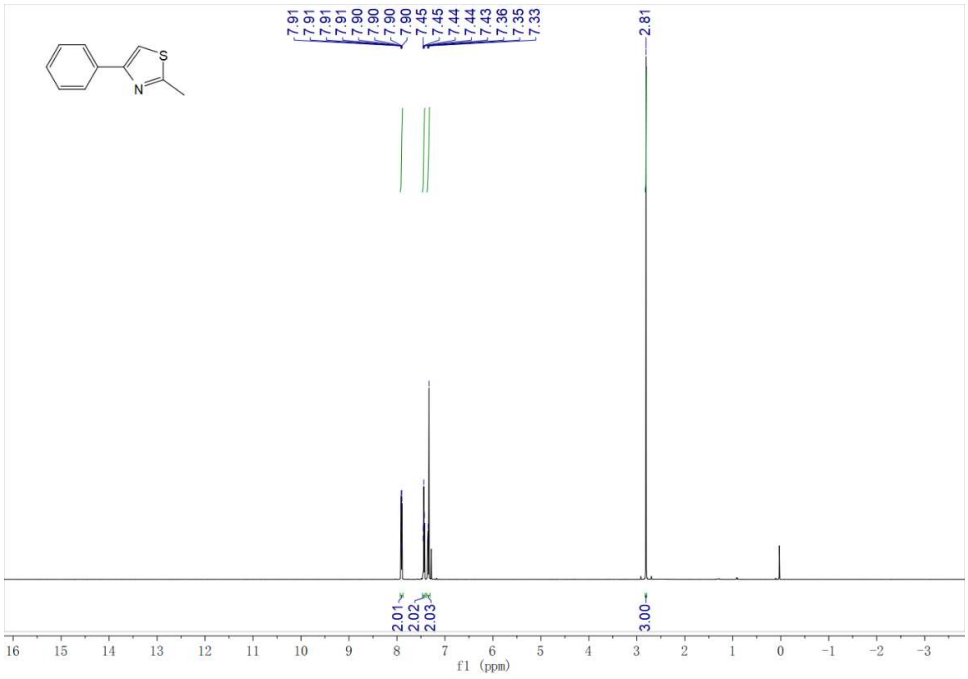


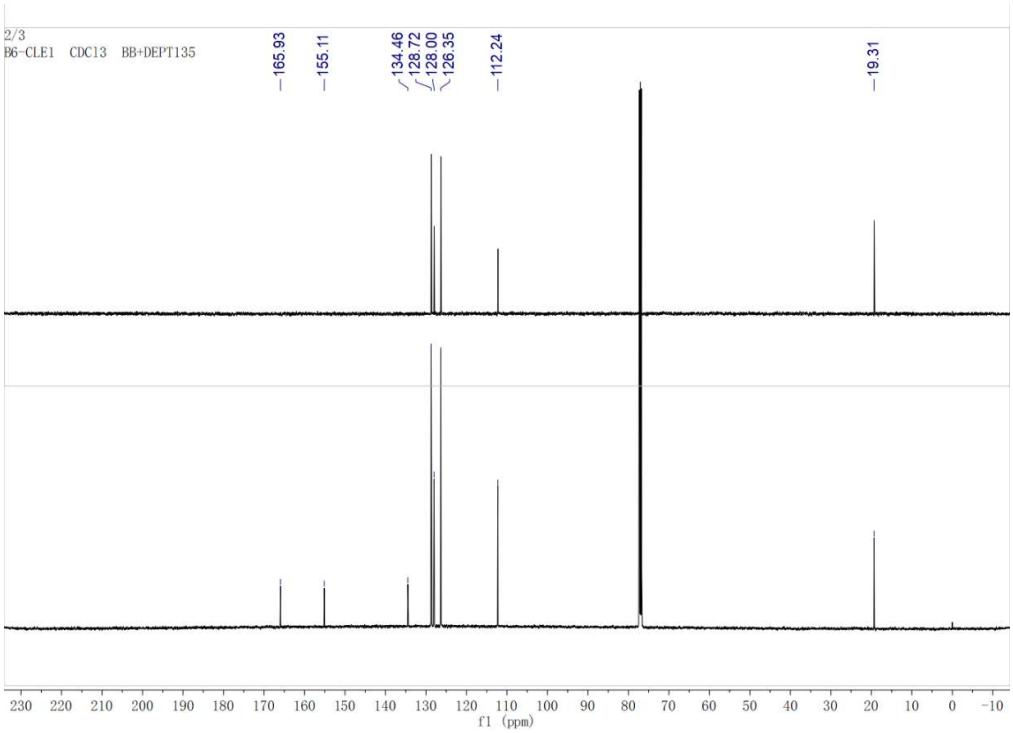
4-Phenylthiazol-2-amine (5d)



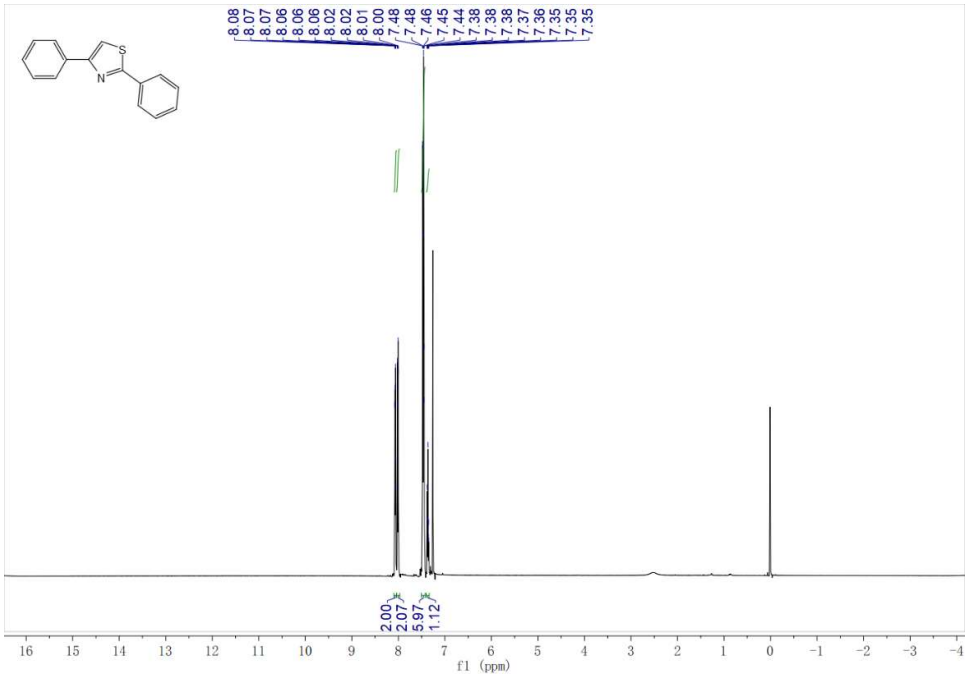


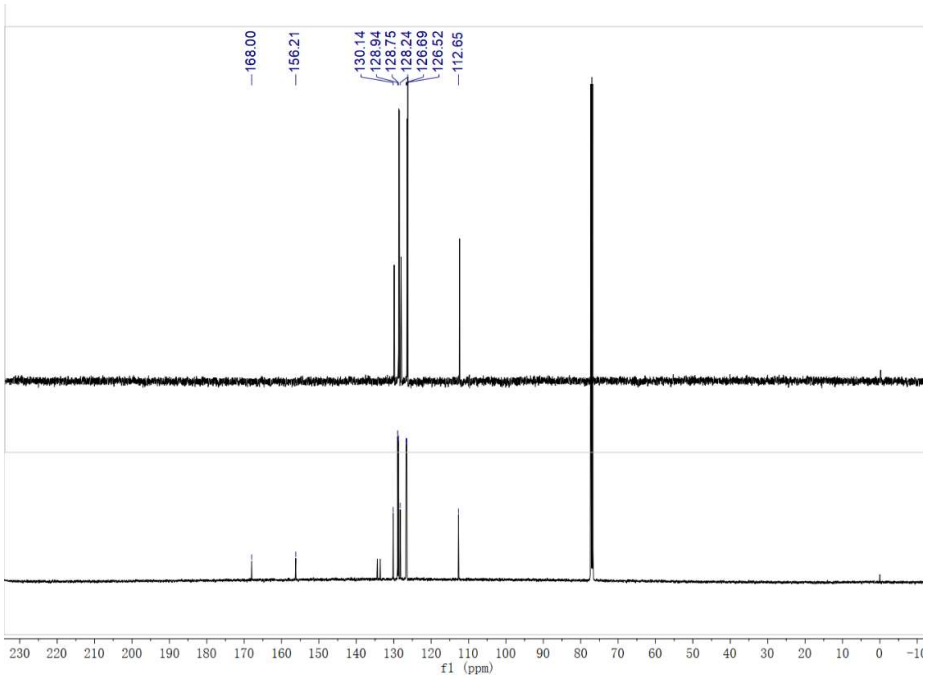
2-Methyl-4-phenylthiazole (5e)





2,4-Diphenylthiazole (5f)





2-Phenylimidazo[2,1-a]isoquinoline (5g)