

Supporting Information
Synthesis of Trifluoromethyl and Ester Group Substituted α -Carbolines
via Iron-Catalyzed Tandem Cyclization Reaction

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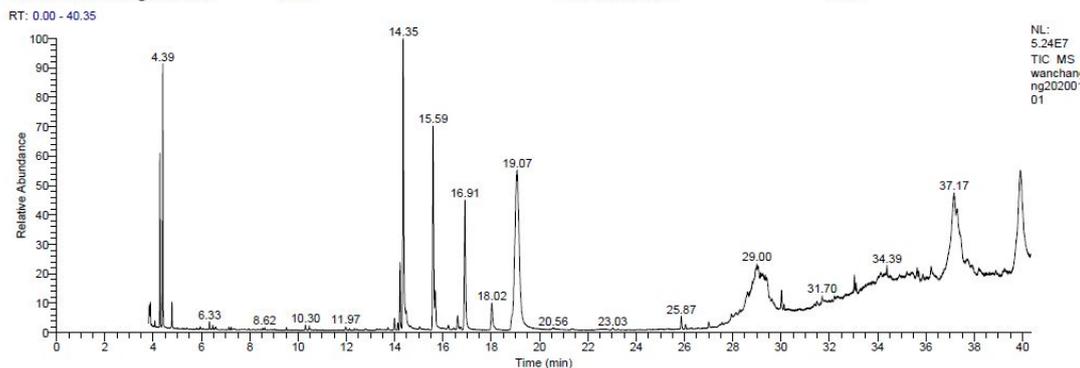
*(a College of Chemistry and Chemical Engineering, Jiangxi Normal University, Nanchang 330022, China;
b Department of Chemistry, University of Science and Technology of China, Hefei 230026, China; c School of
Metallurgy and Chemical Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, China.)*

GC-MS spectrum	S2-S3
NMR spectrum of substrates	S4-S12
NMR spectrum of products	S13-S58

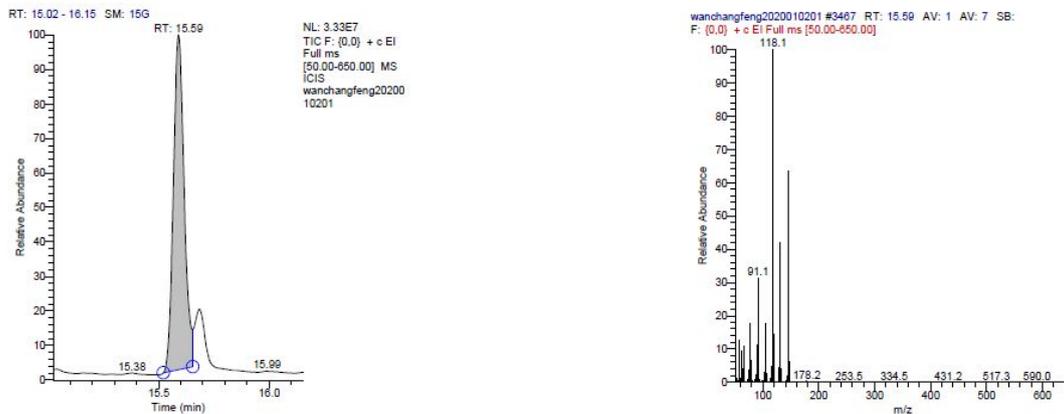
GC-MS spectrum for control experiment A:

My Qual XReport

Data File:	wanchangfeng2020010201	Original Data Path:	E:\DATA2019\wanchangfeng
Current Data Path:	E:\DATA2019\wanchangfeng	Sample Type:	Unknown
Sample ID:	1	Sample Name:	wanchangfeng010201
Operator:	ISQ140444	Acquisition Date:	01/02/20 10:20:20 PM
Run Time(min):	36.54	Comments:	
Vial:	6	Injection Volume(μl):	1.00
Scans:	10746	Low Mass(m/z):	50
High Mass(m/z):	650	Sample Volume(μl):	0.00
Sample Weight:	0.00	ISTD Amount:	0.000
Calibration Level:		Dilution Factor:	1.00
Instrument Method:	E:\Method\TG-5MS 40MIN.meth	Original Processing Method:	
Current Processing Method:	N/A	Calibration File:	N/A

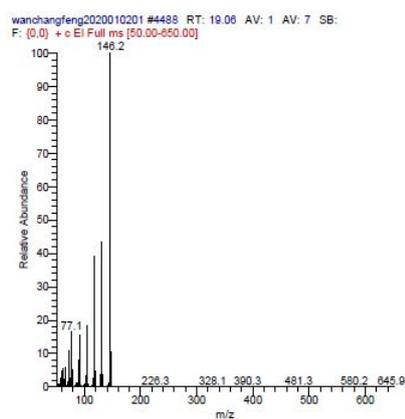
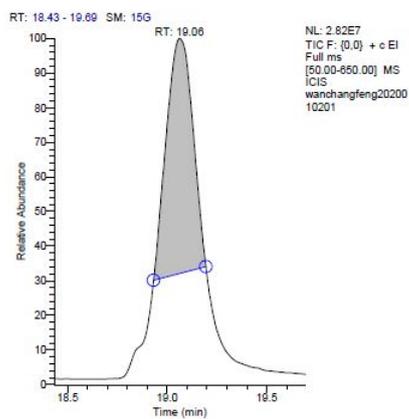


1a



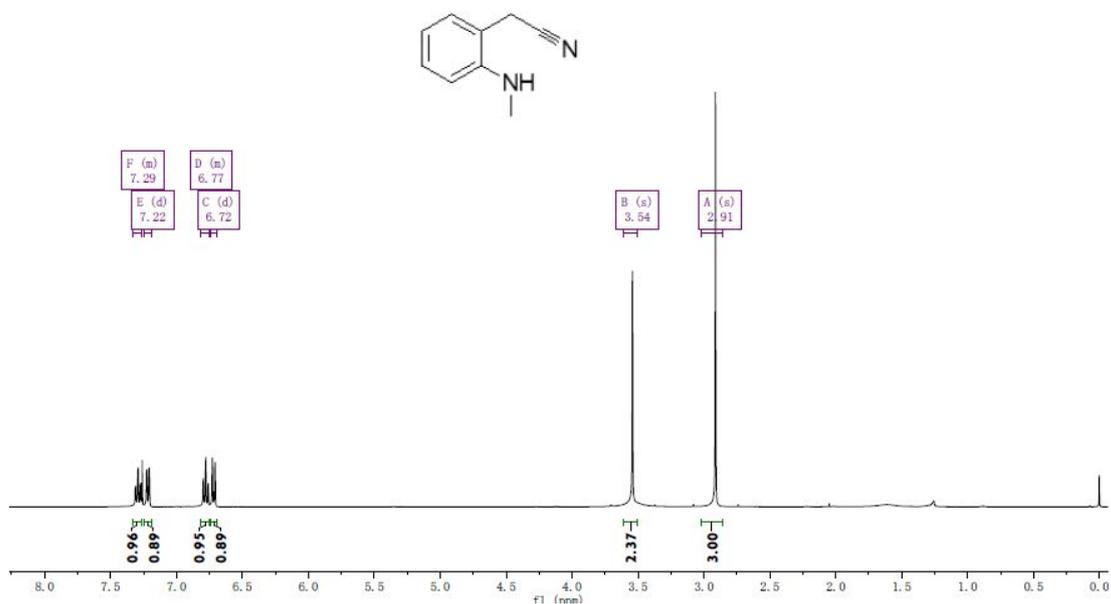
RT	SI	RSI	Compound Name	Molecular Formula	Library	Area	Area %
15.59	759	762	2-Methyl-5-(4-methylphenyl)tetrazole	C9H10N4	mainlib	109777029.68	10.92
15.59	758	791	Cinnoline, 1,2-dihydro-2-methyl-	C9H10N2	mainlib	109777029.68	10.92
15.59	783	794	1H-1,3,2-Benzodiazaborole, 2-ethyl-2,3-dihydro-	C8H11BN2	mainlib	109777029.68	10.92

Intermediate A

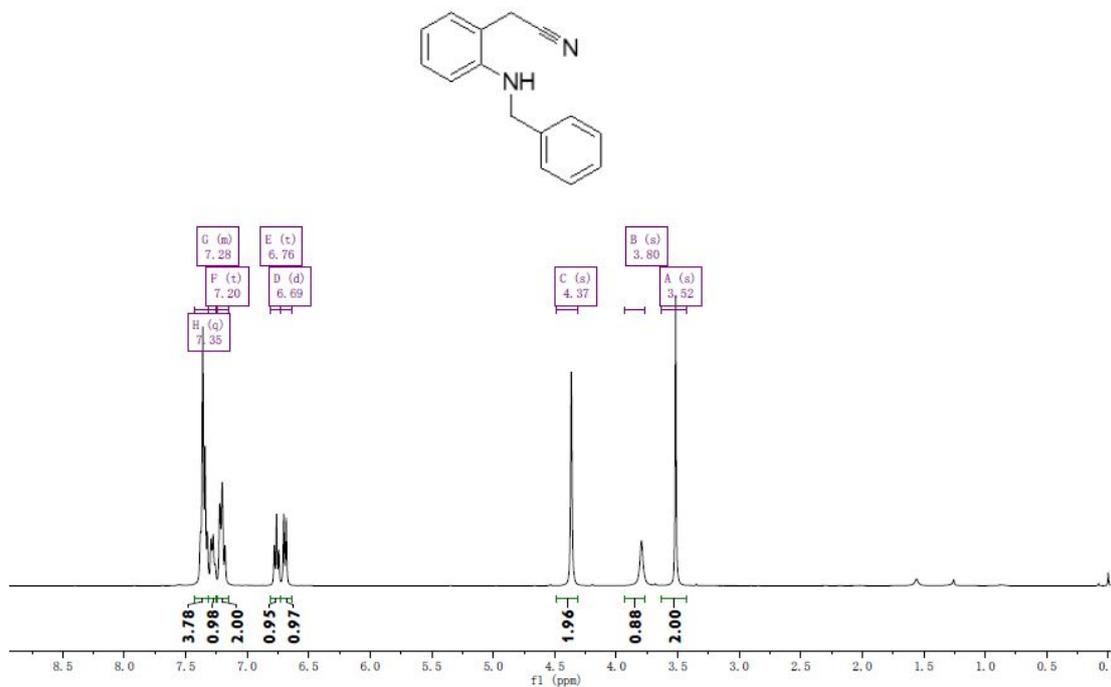


RT	SI	RSI	Compound Name	Molecular Formula	Library	Area	Area %
19.06	791	792	1H-Indazole, 5,7-dimethyl-	C9H10N2	mainlib	174890362.53	17.39
19.06	789	789	1H-Benzimidazole, 5,6-dimethyl-	C9H10N2	mainlib	174890362.53	17.39

2-(2-(methylamino)phenyl)acetonitrile (1a)

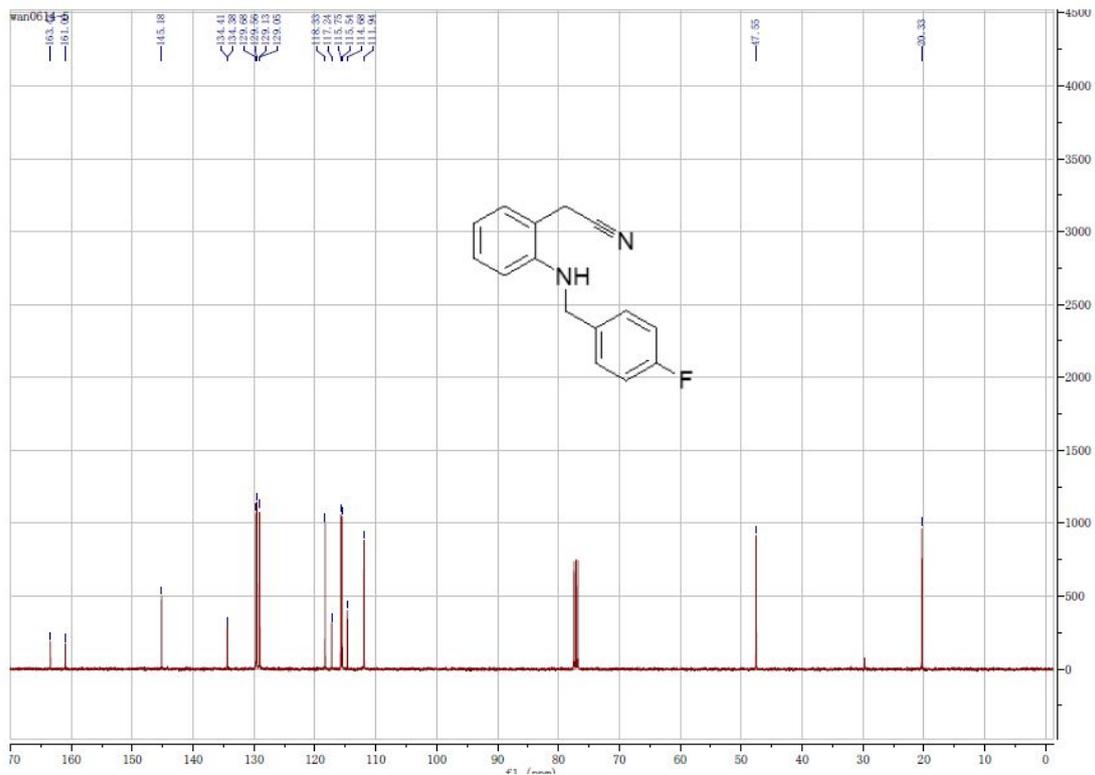
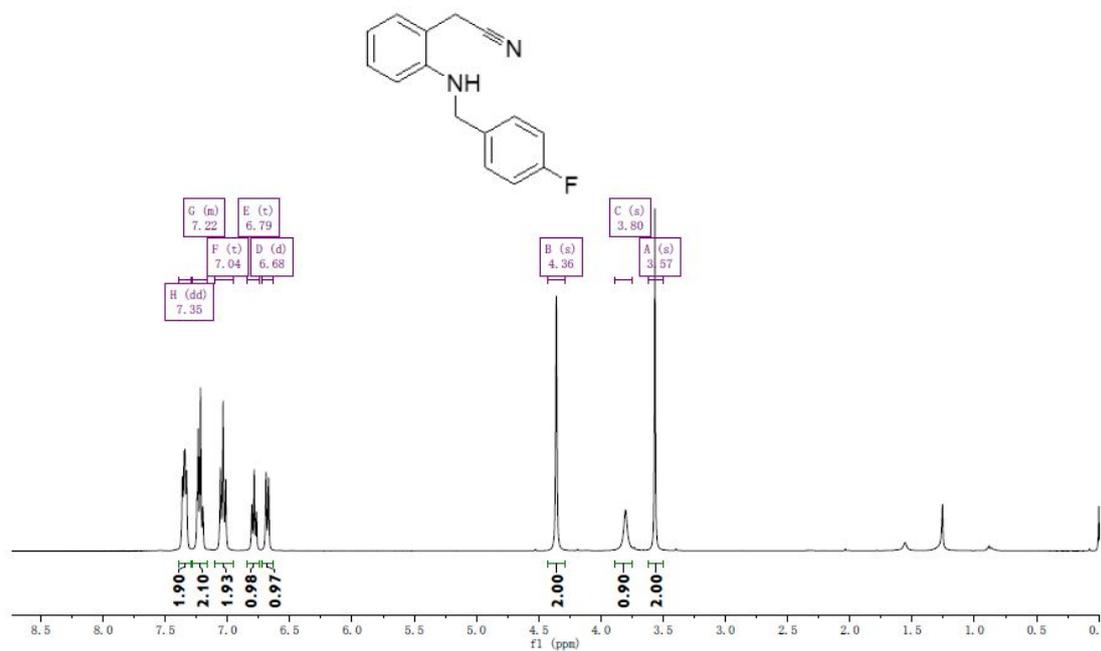


2-(2-(benzylamino)phenyl)acetonitrile (1p)

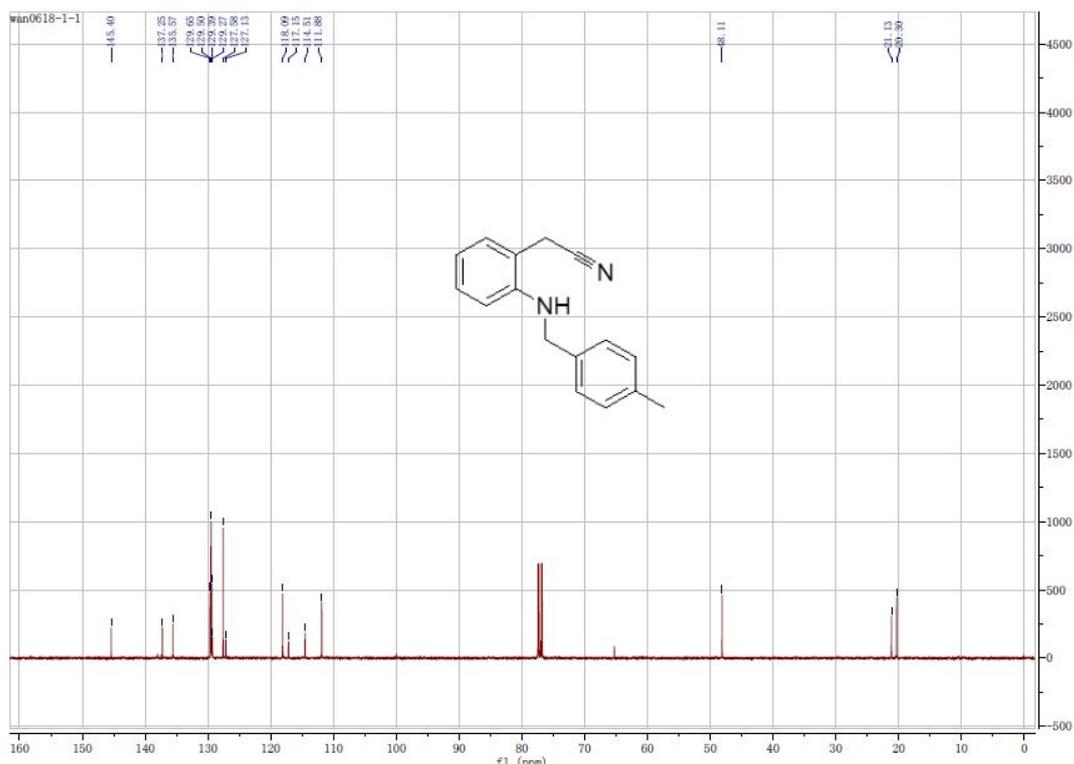


2-(2-(4-fluorobenzylamino)phenyl)acetonitrile (1q)

wcf0614-5

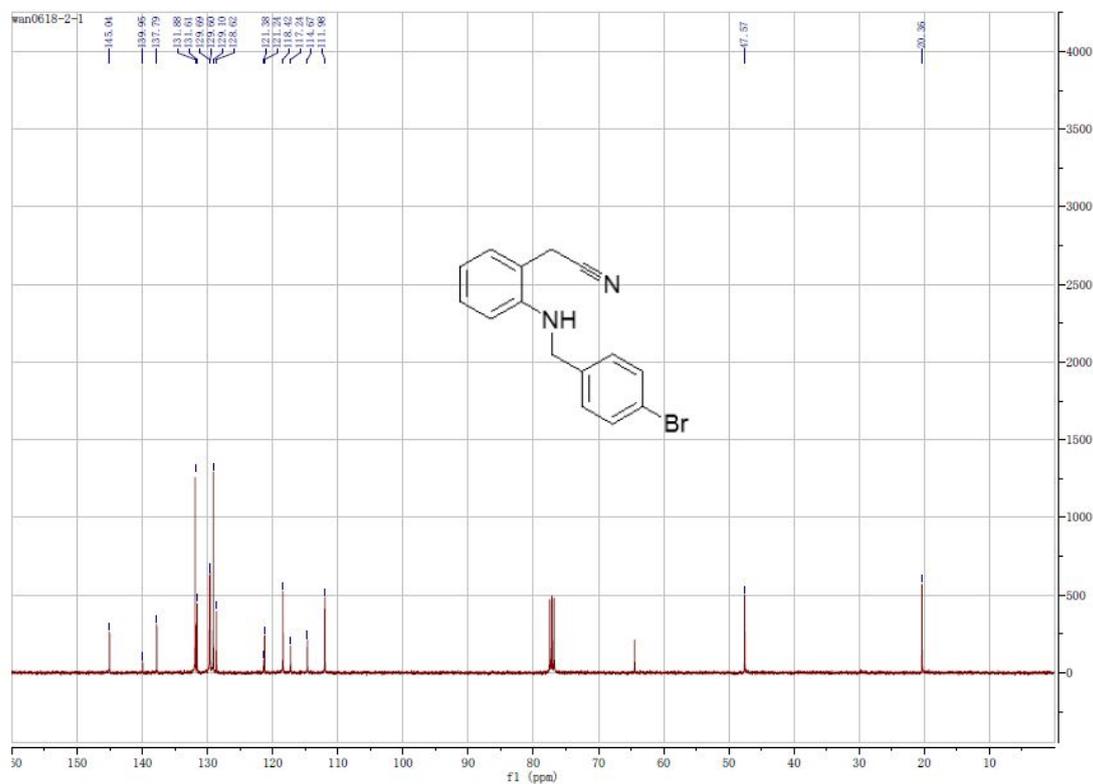
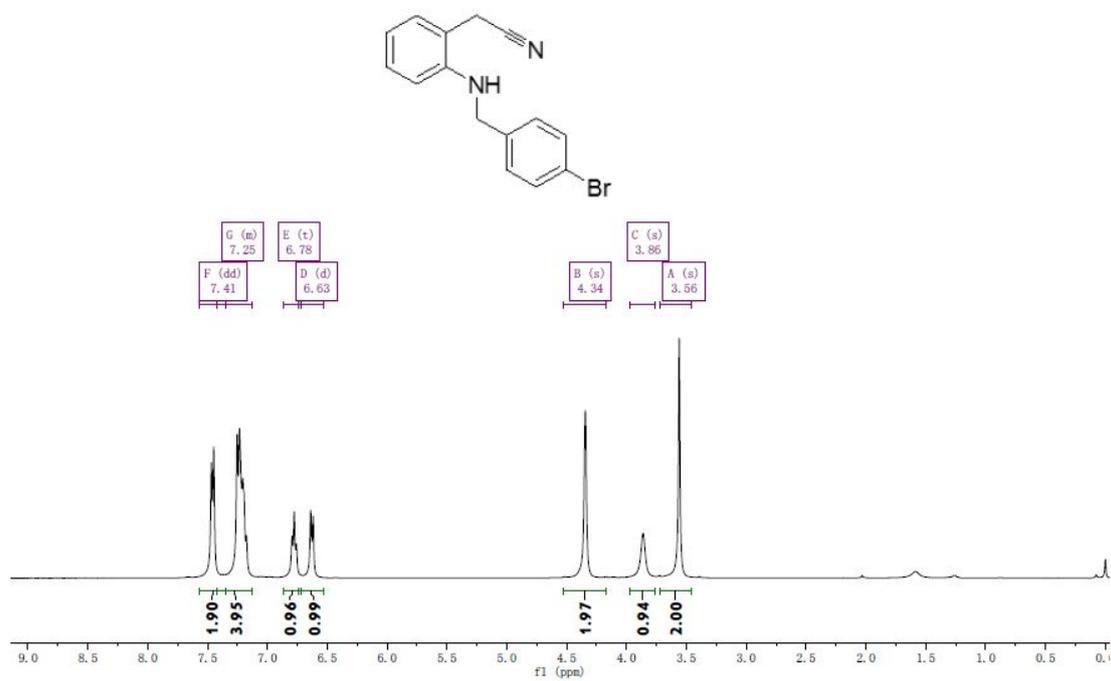


2-(2-(4-methylbenzylamino)phenyl)acetonitrile (1r)

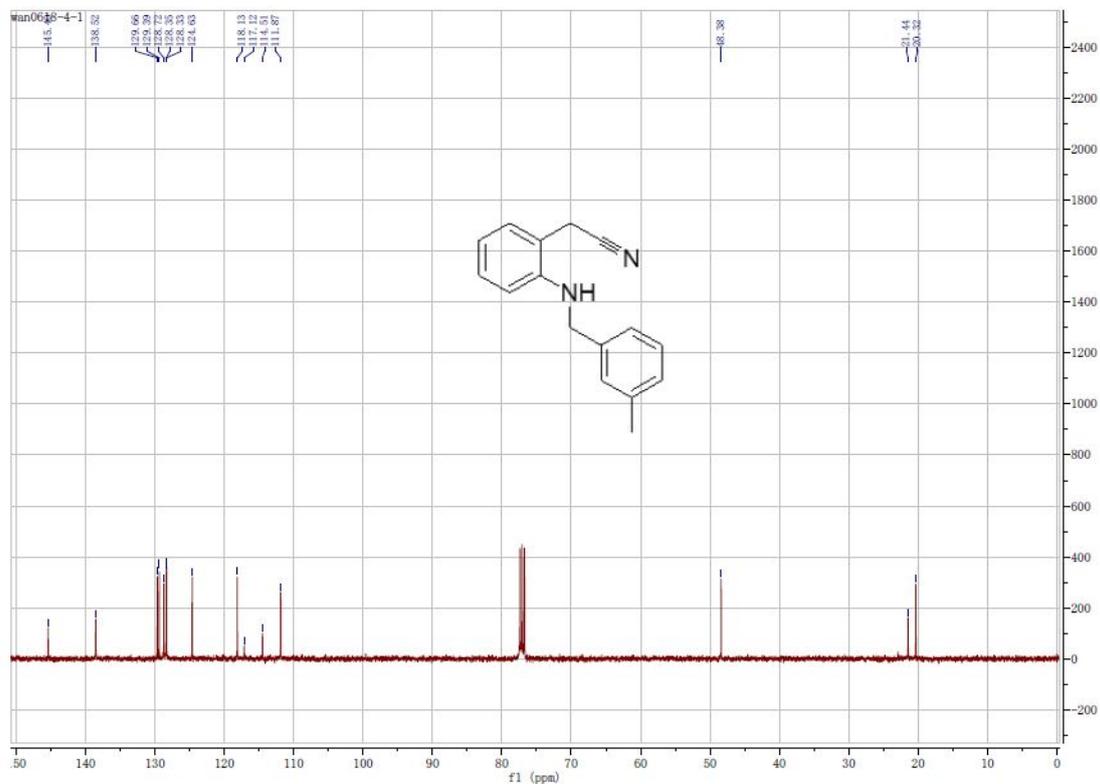
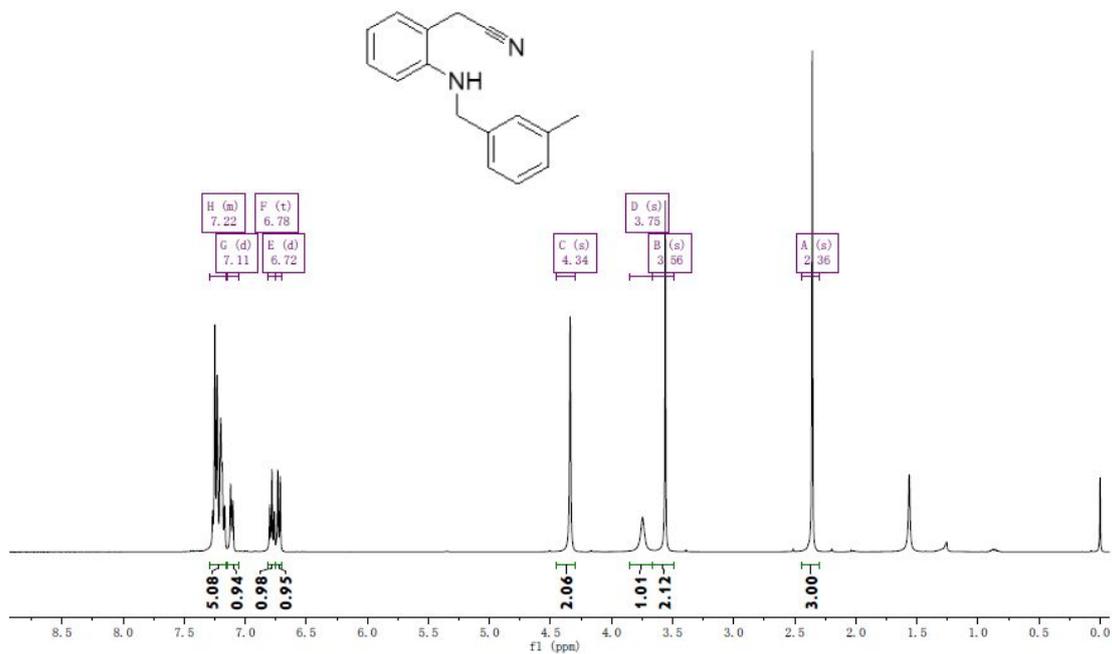


2-(2-(4-bromobenzylamino)phenyl)acetonitrile (1s)

wan0618-2

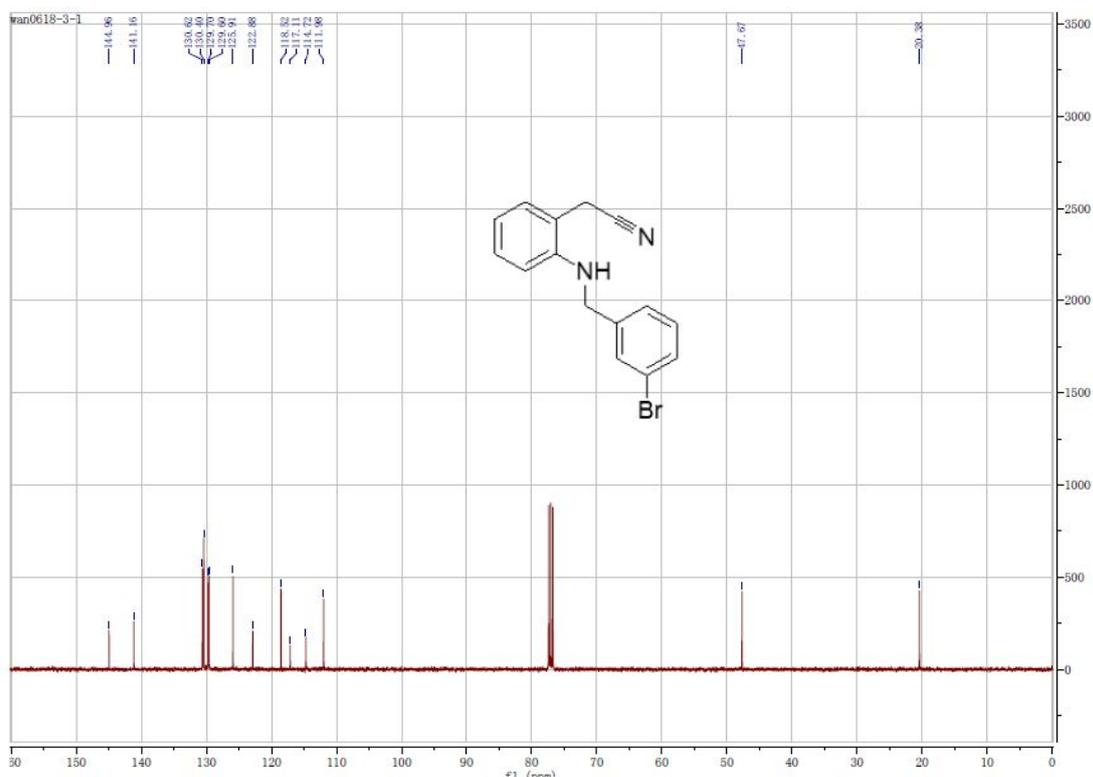
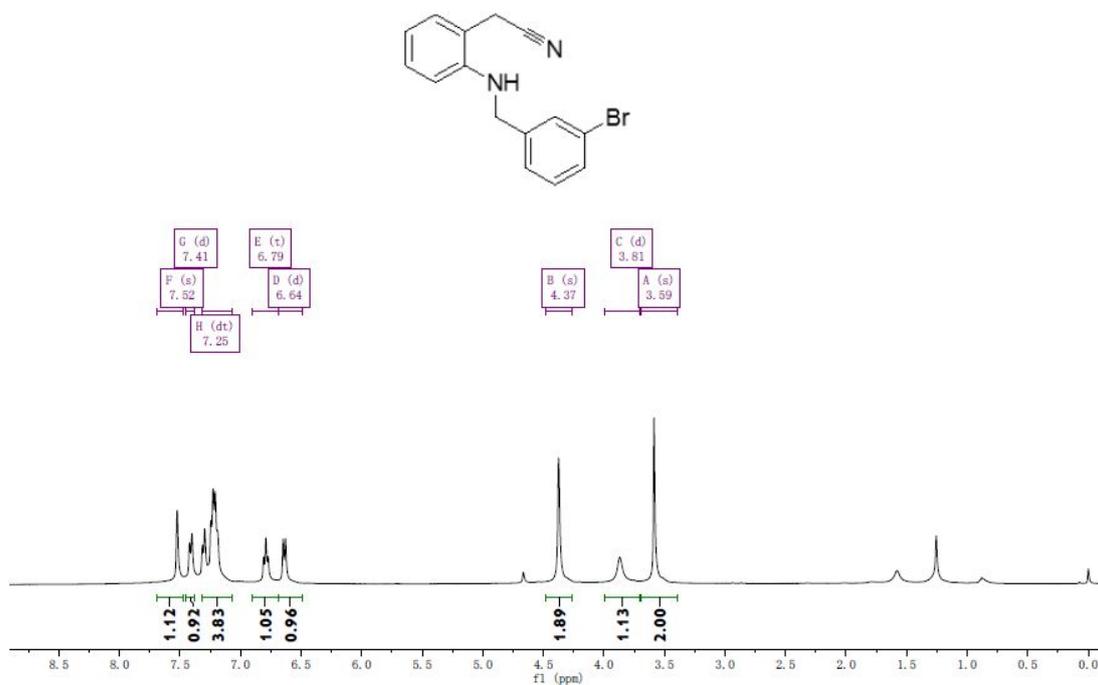


2-(2-(3-methyl benzylamino)phenyl)acetonitrile (1t)

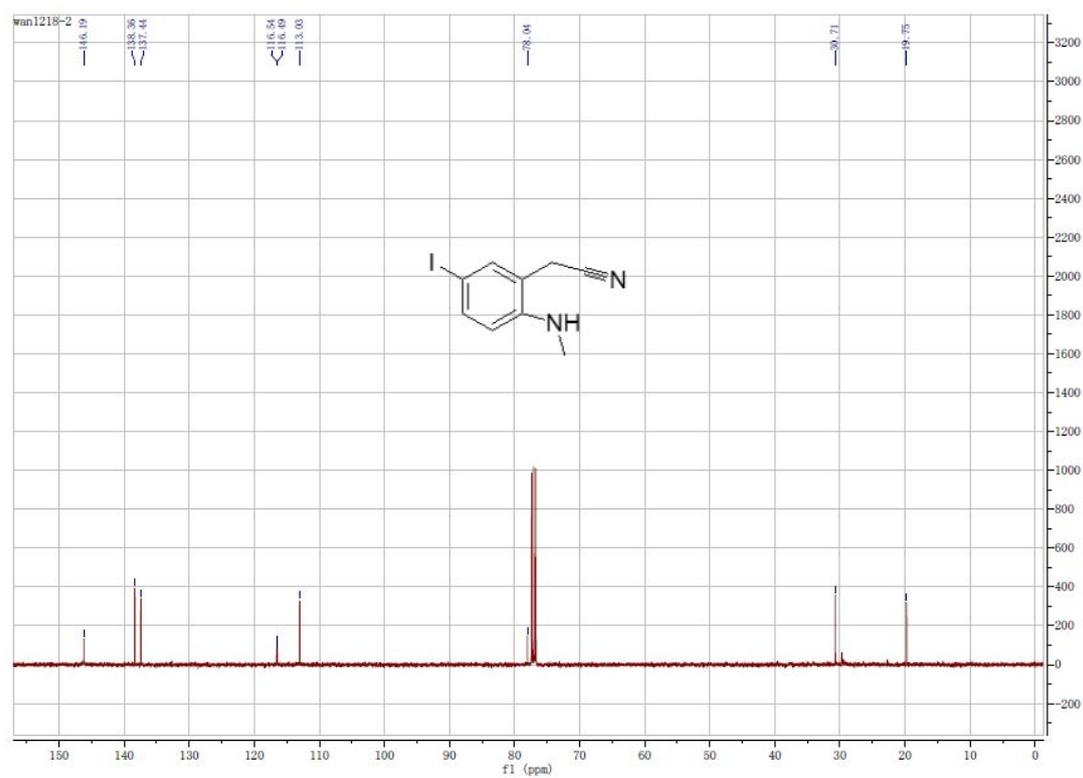
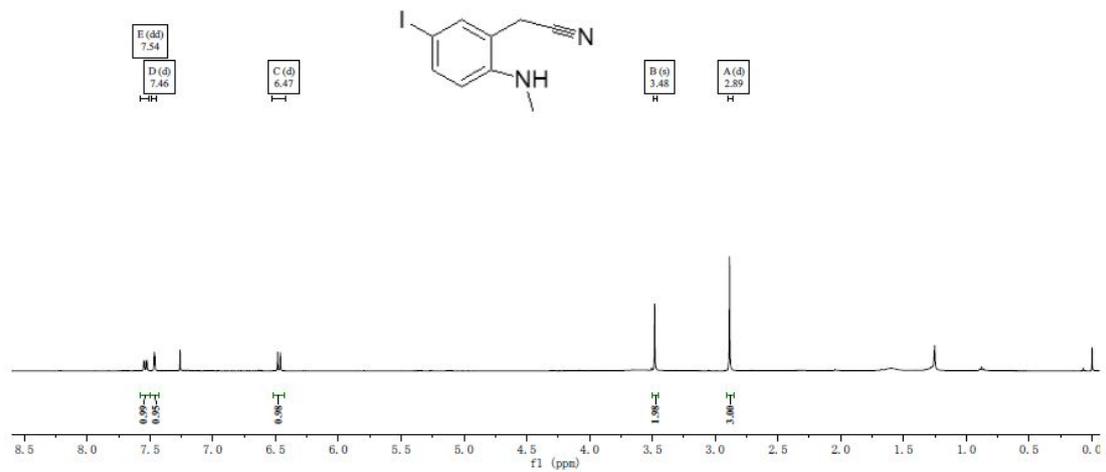


2-(2-(3-bromo benzylamino)phenyl)acetonitrile (1g)

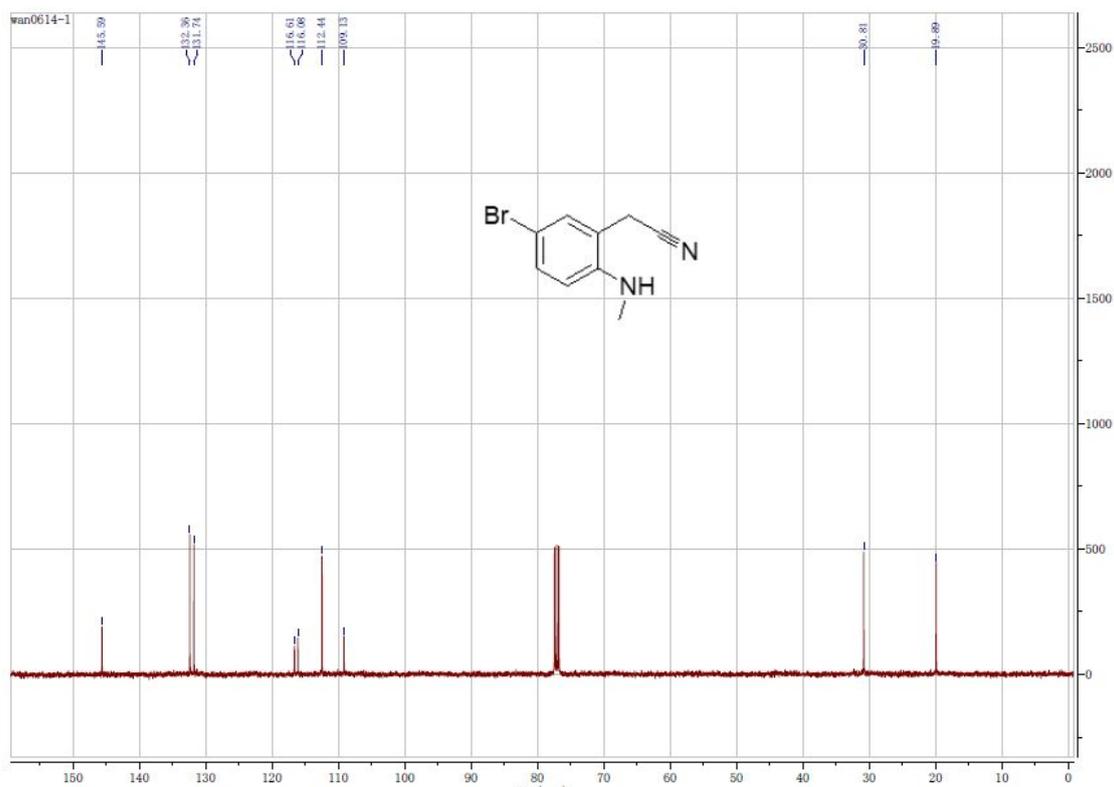
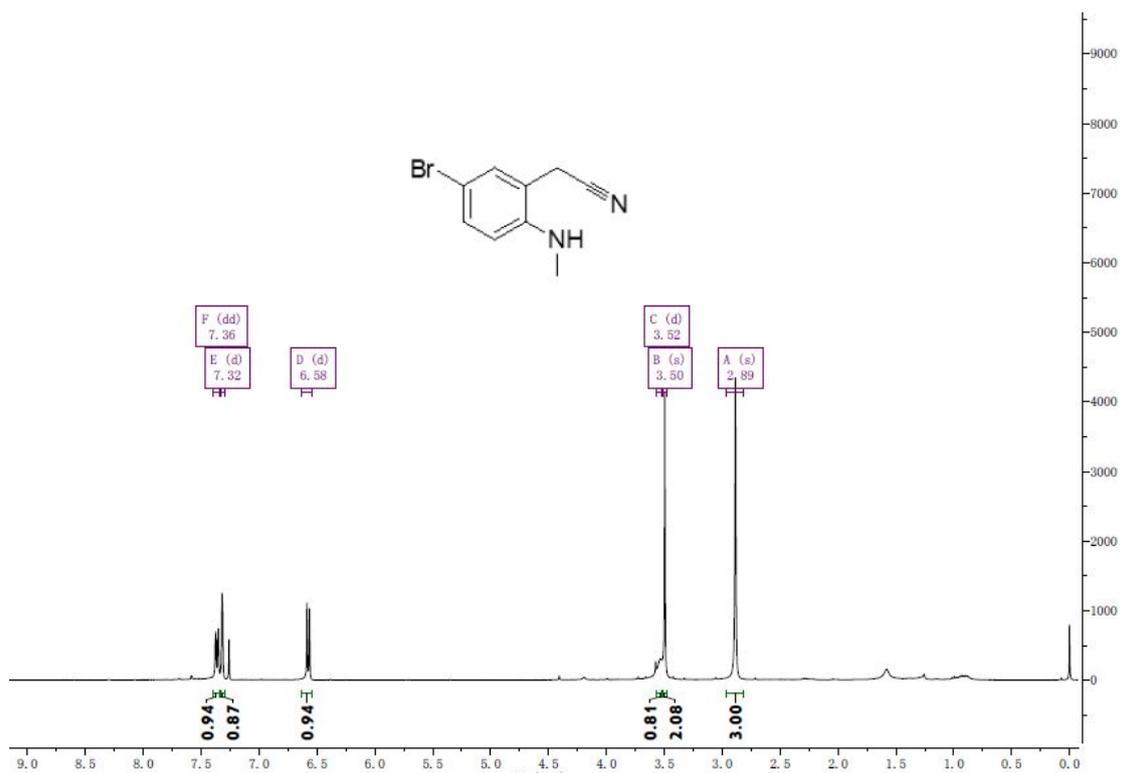
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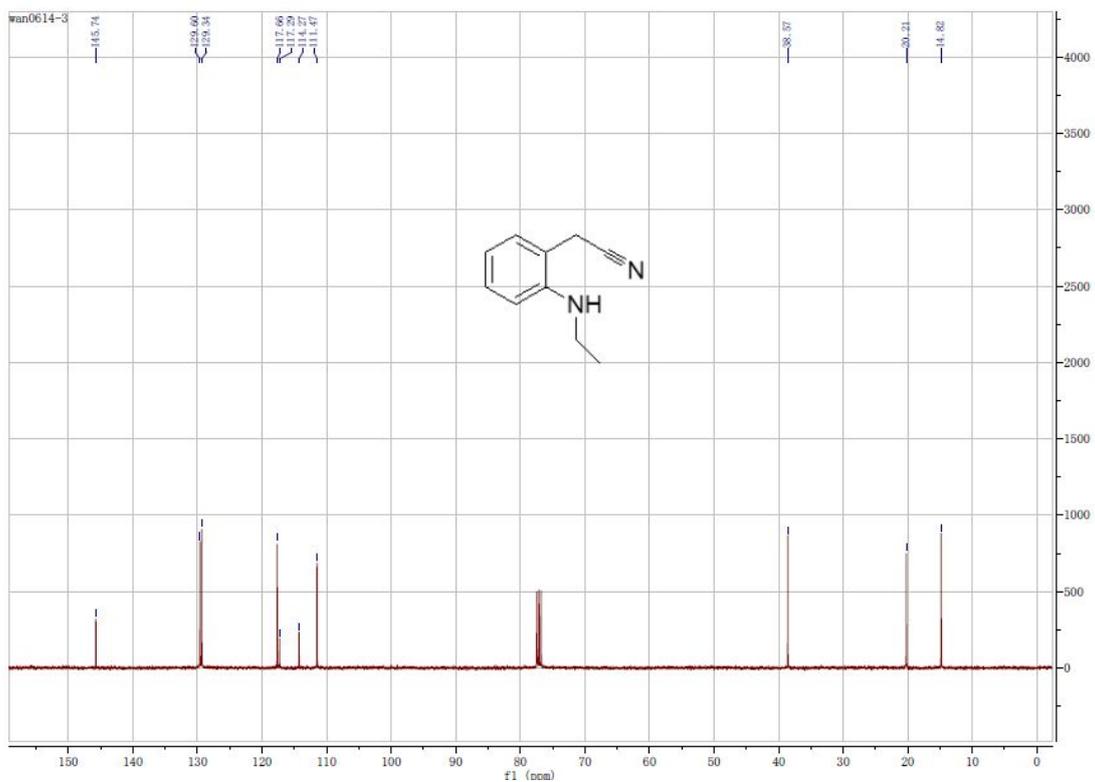
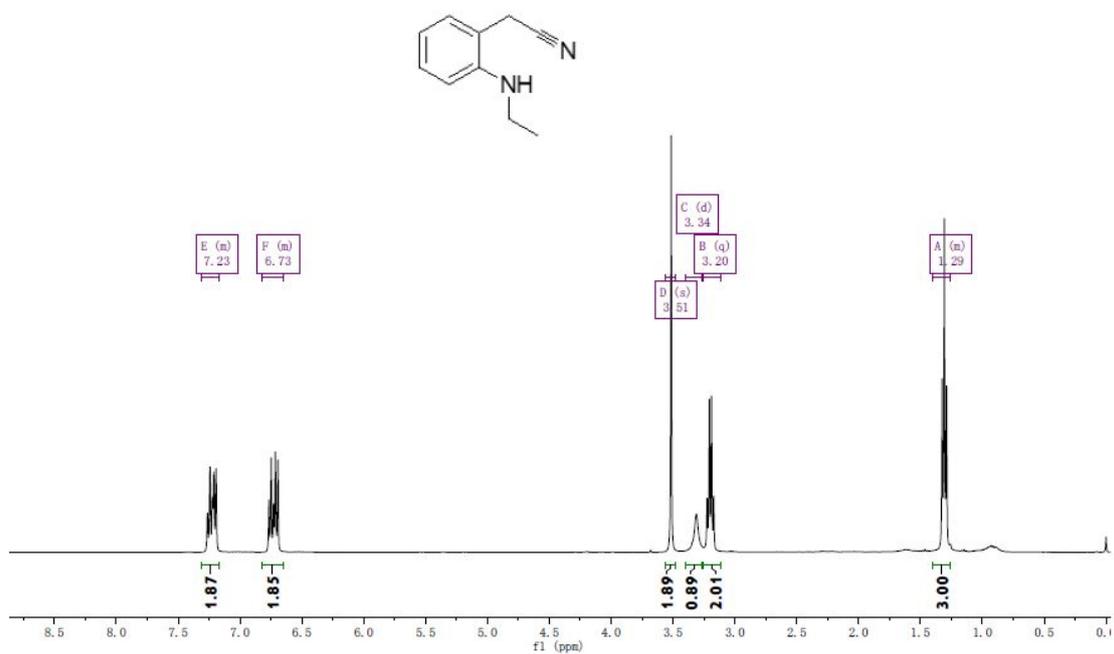
2-(5-iodo-2-(methylamino)phenyl)acetonitrile (1l)



2-(5-bromo-2-(methylamino)phenyl)acetonitrile (1m)

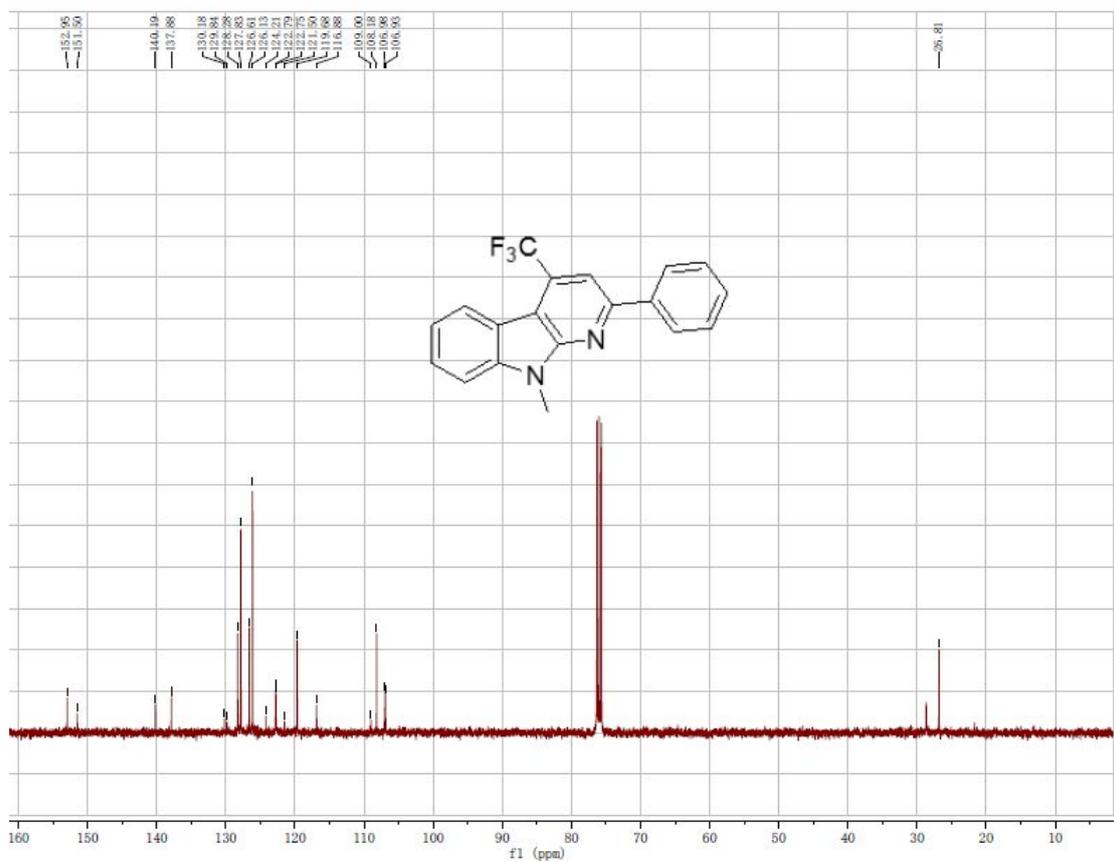
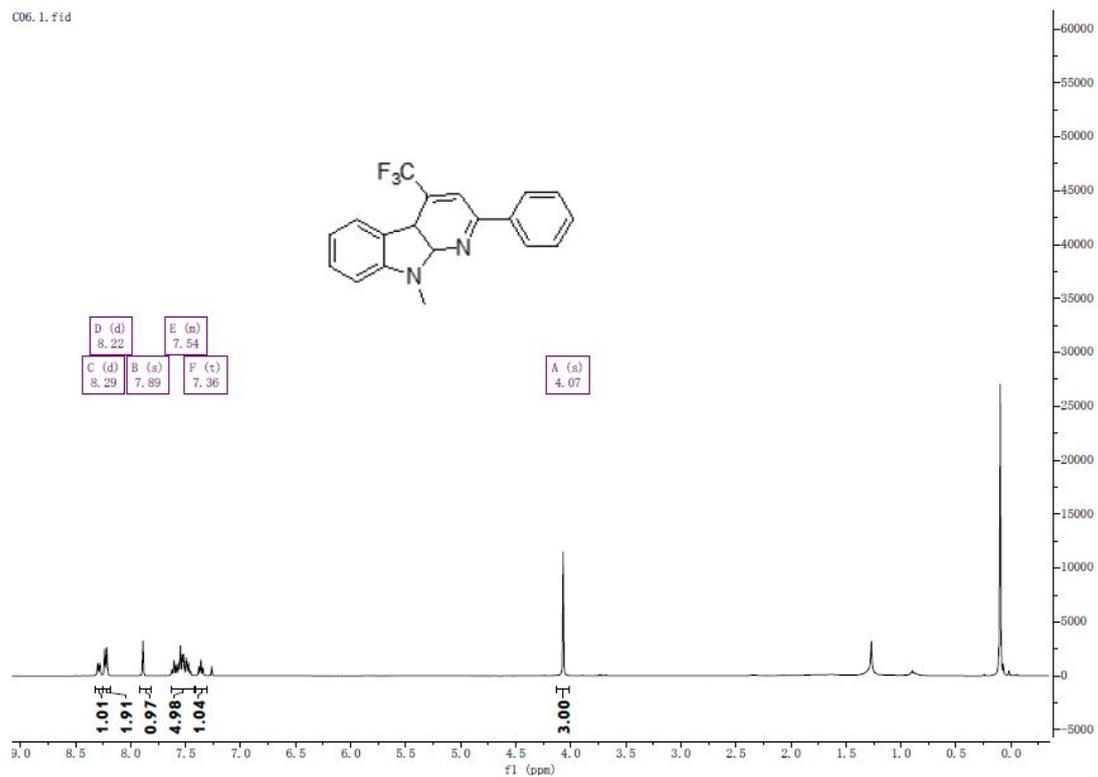


2-(2-(ethylamino)phenyl)acetonitrile (1n)

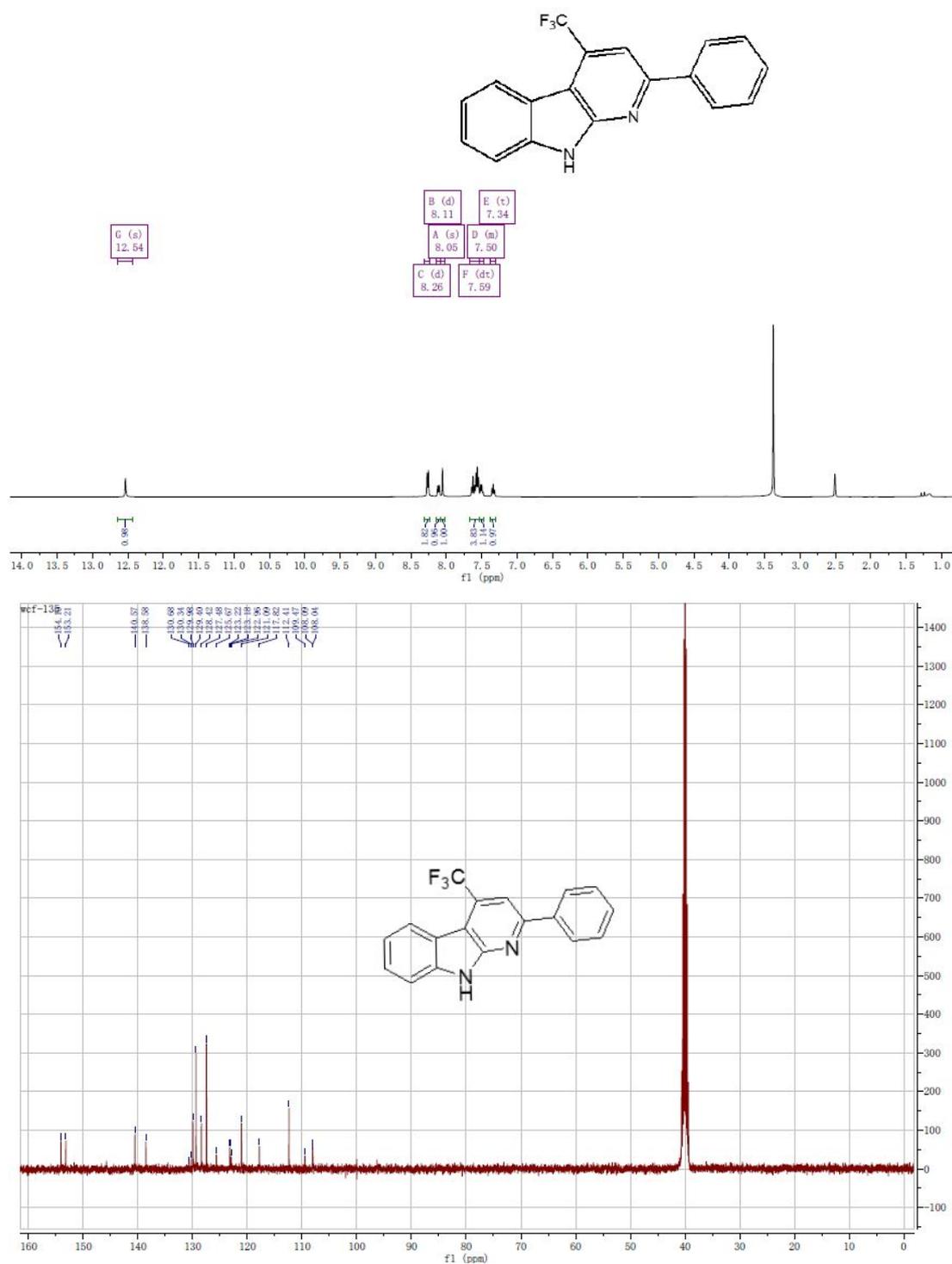


9-methyl-2-phenyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3a)

006.1.fid

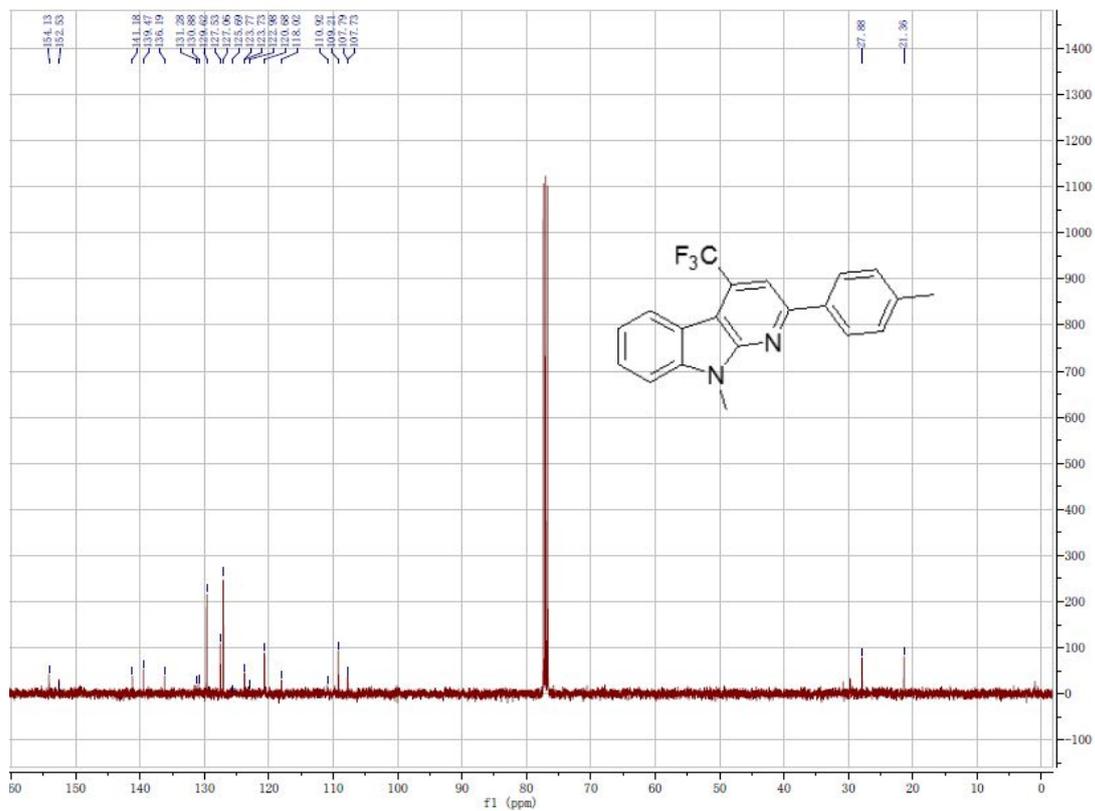
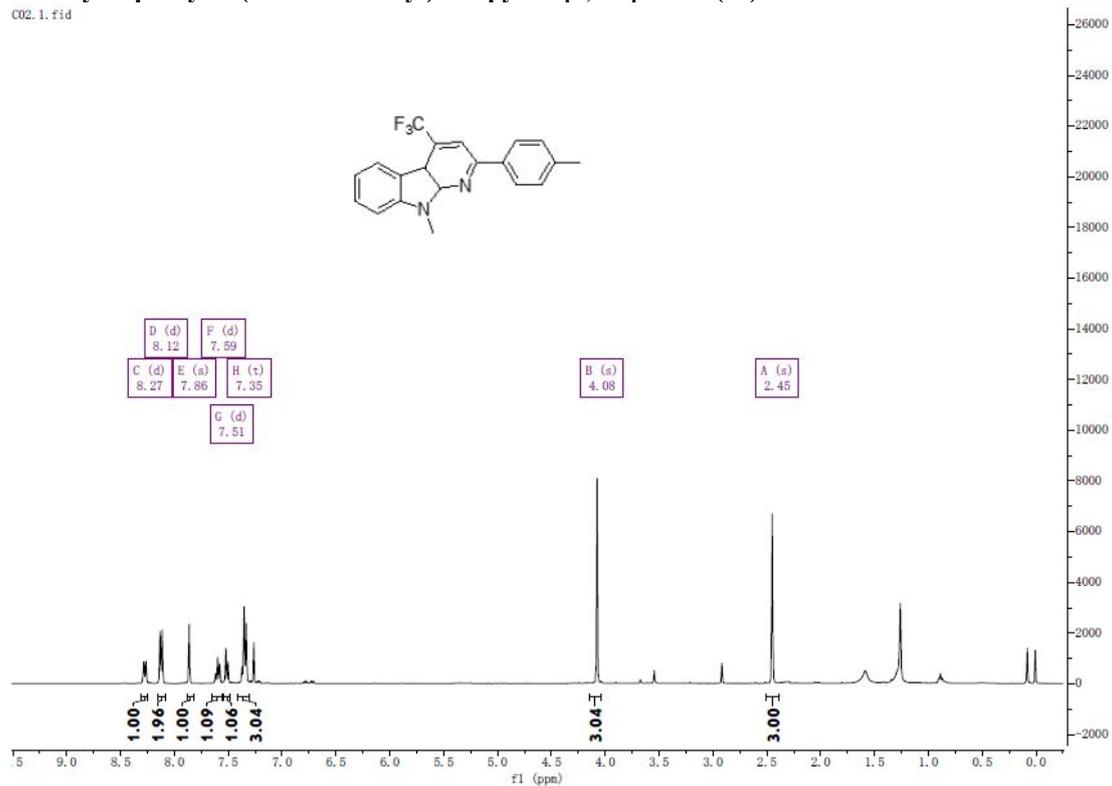


2-phenyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3b)

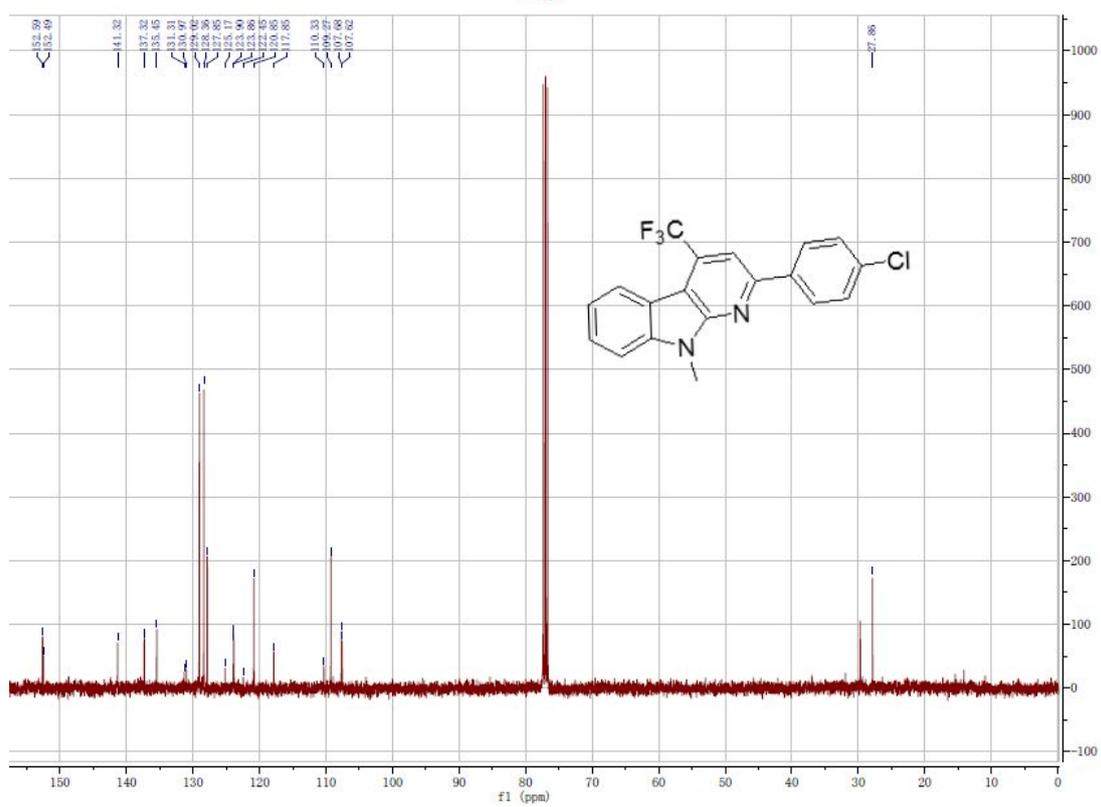
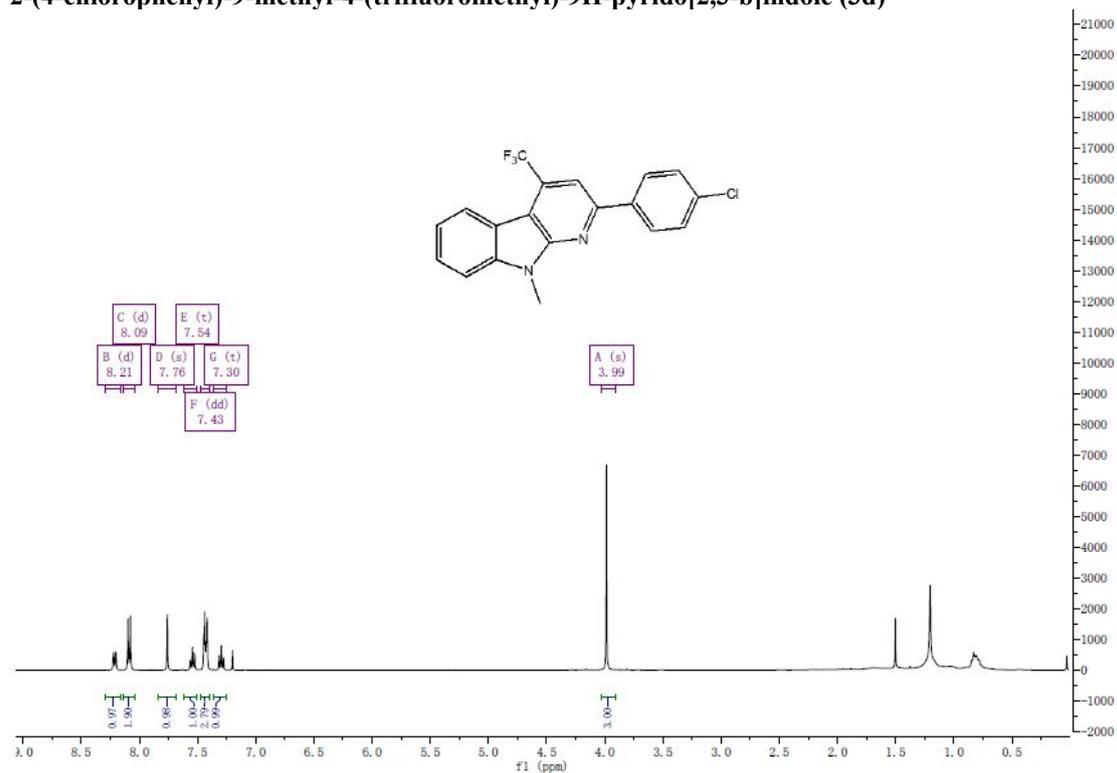


9-methyl-2-p-tolyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3c)

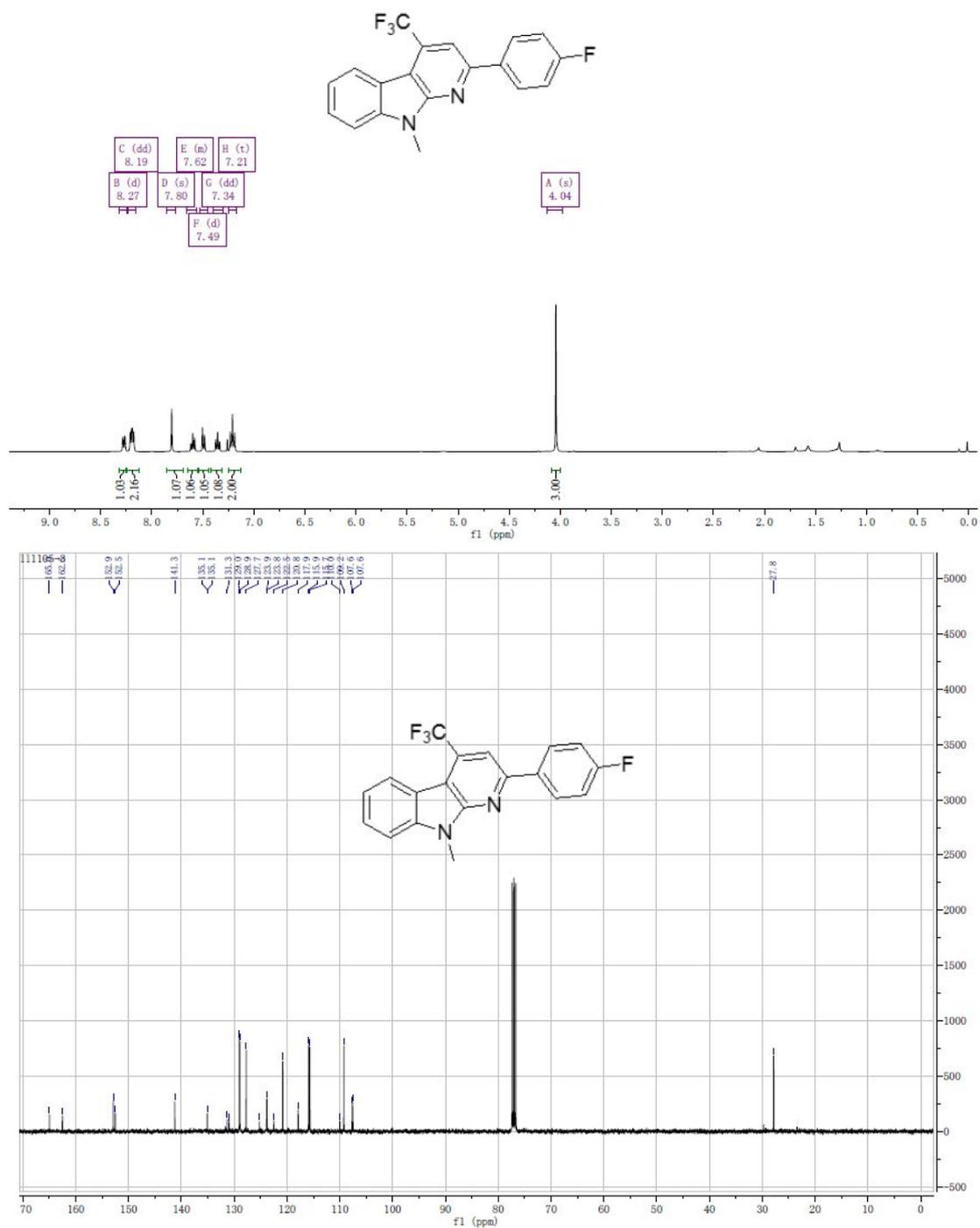
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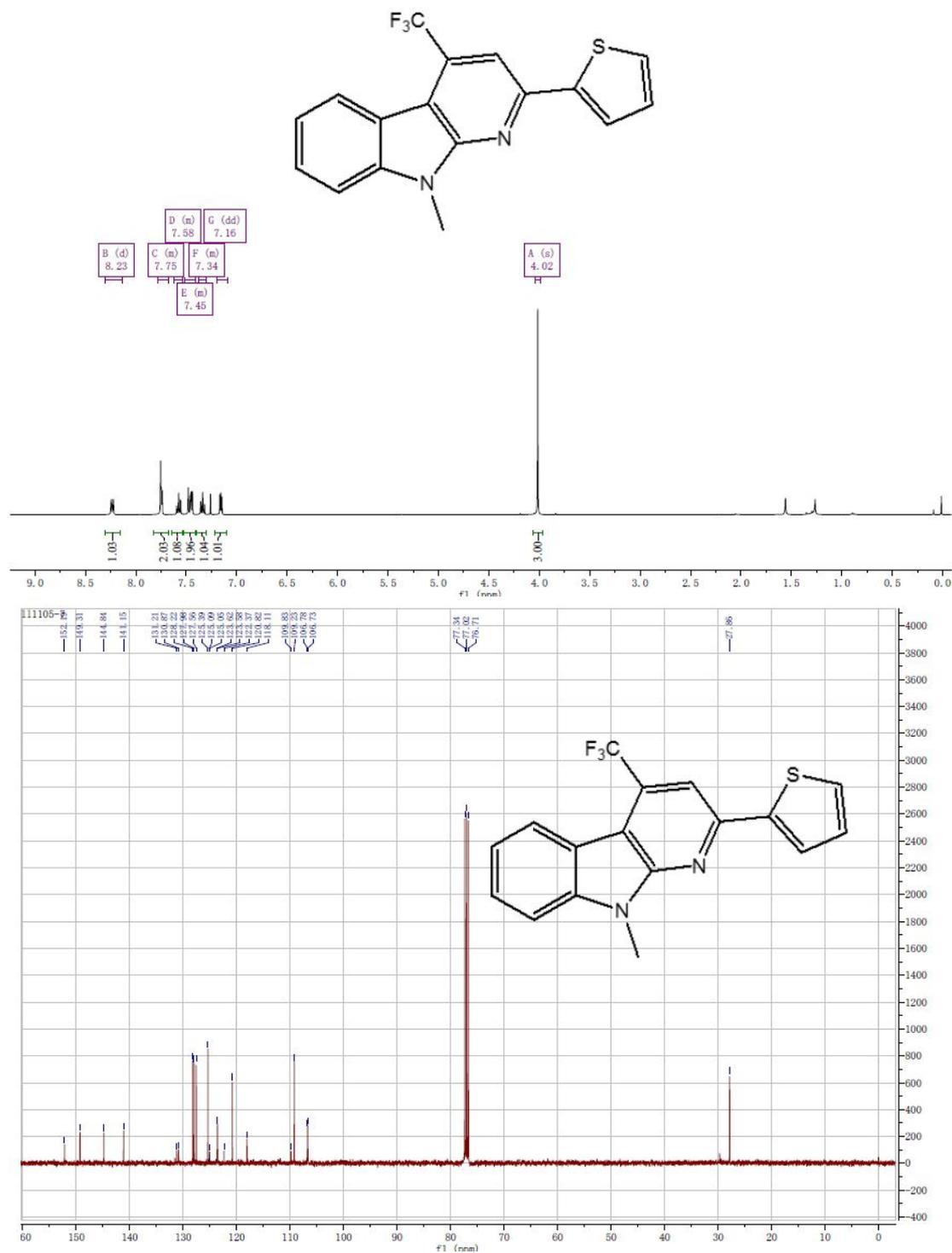
2-(4-chlorophenyl)-9-methyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3d)



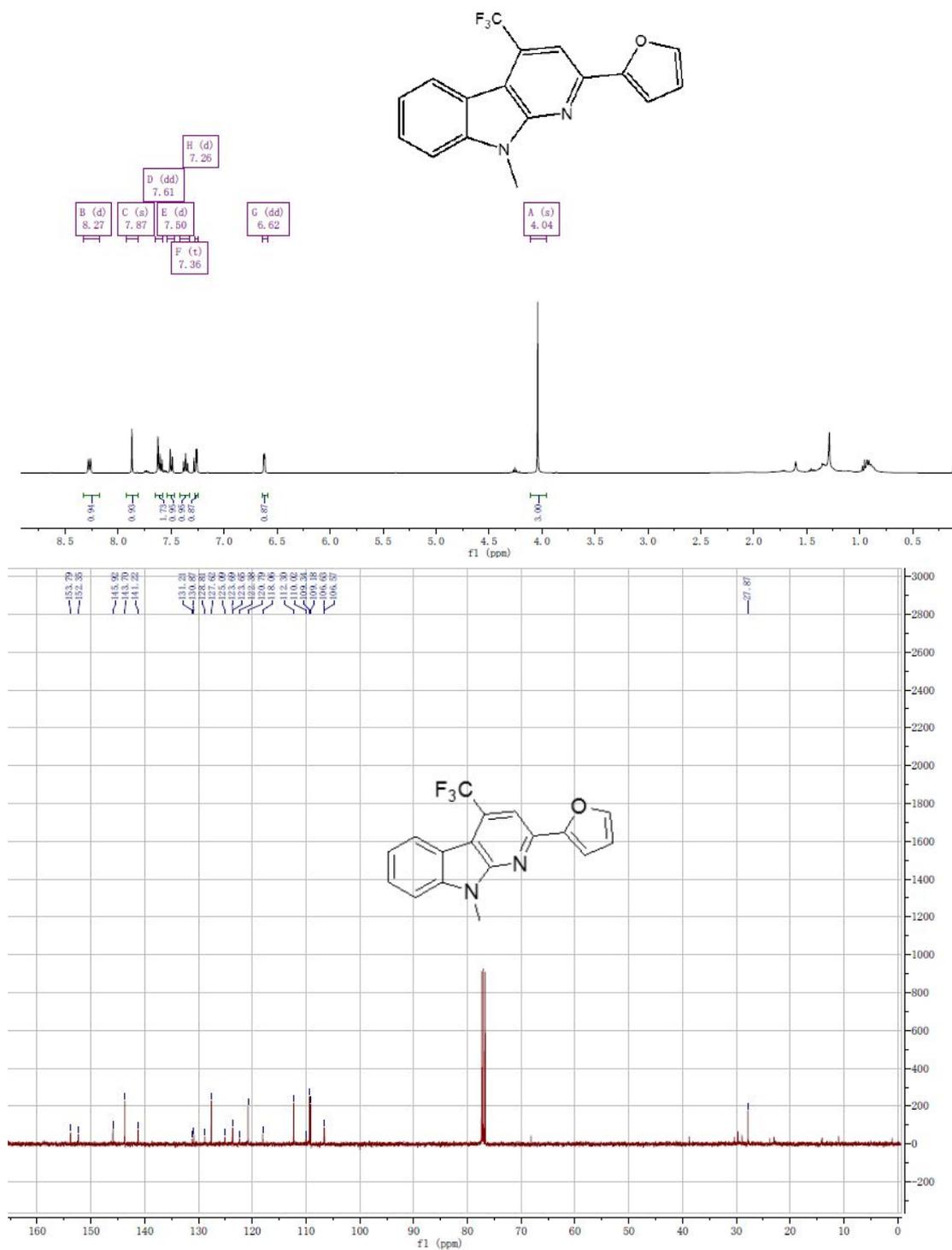
2-(4-fluorophenyl)-9-methyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3e)



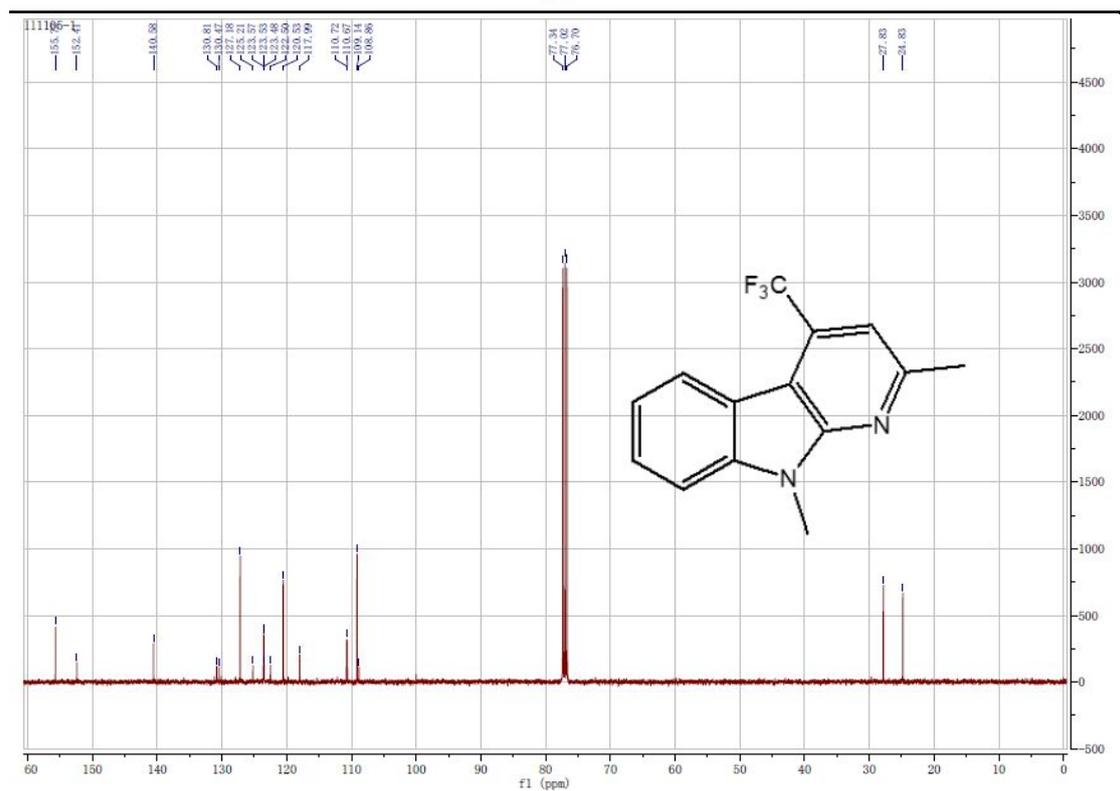
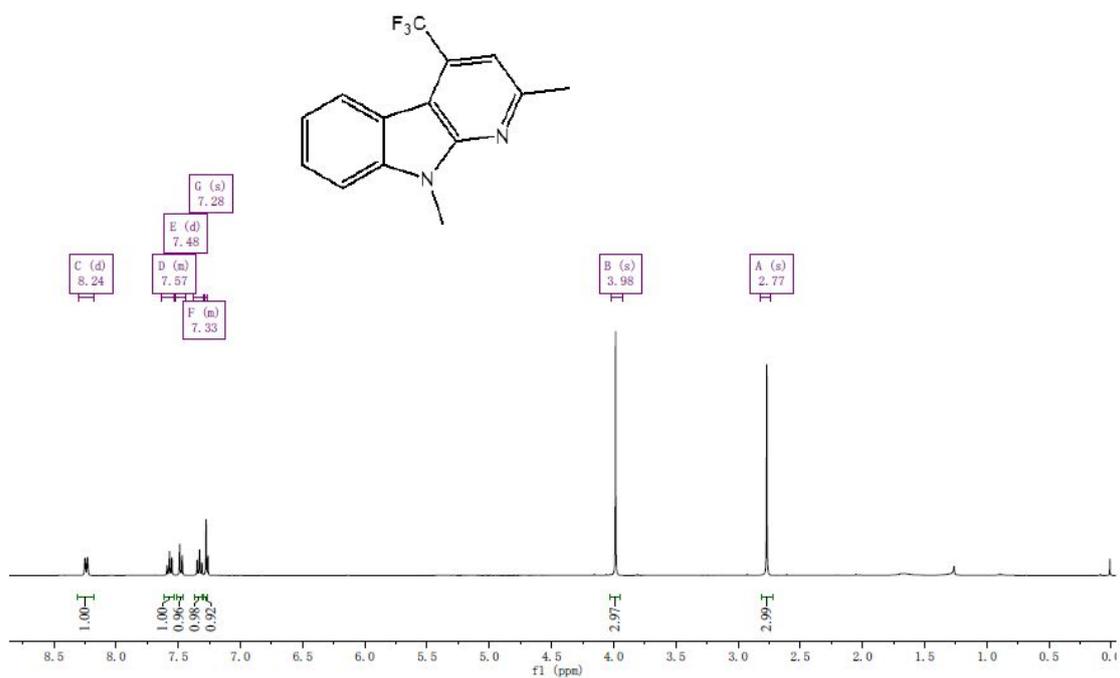
9-methyl-2-(thiophen-2-yl)-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3g)



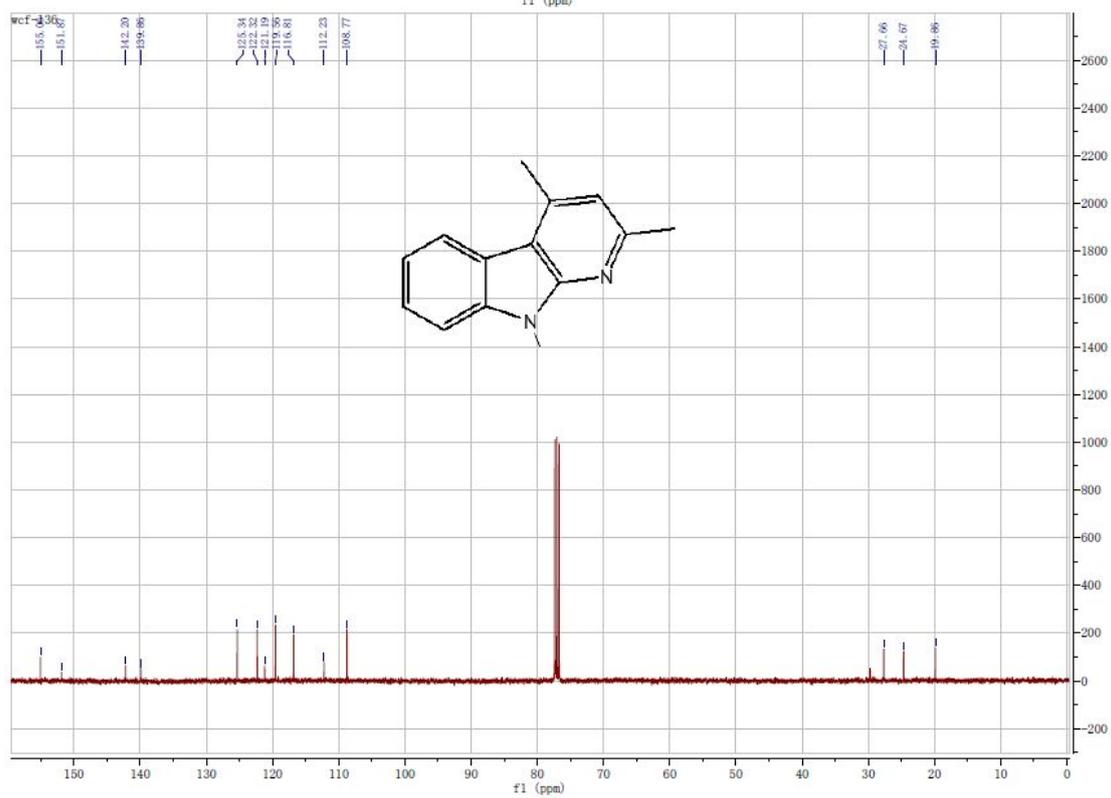
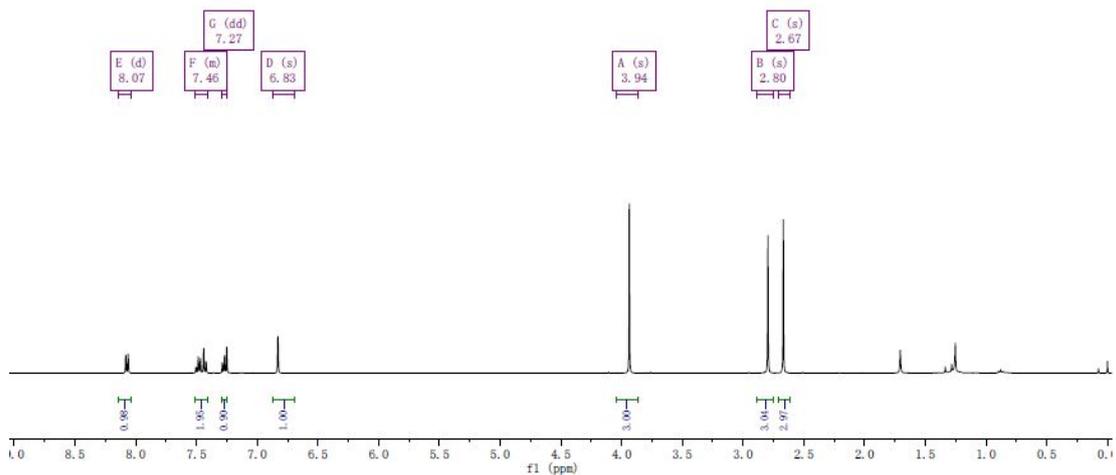
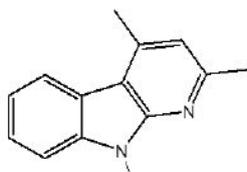
2-(furan-2-yl)-9-methyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3h)



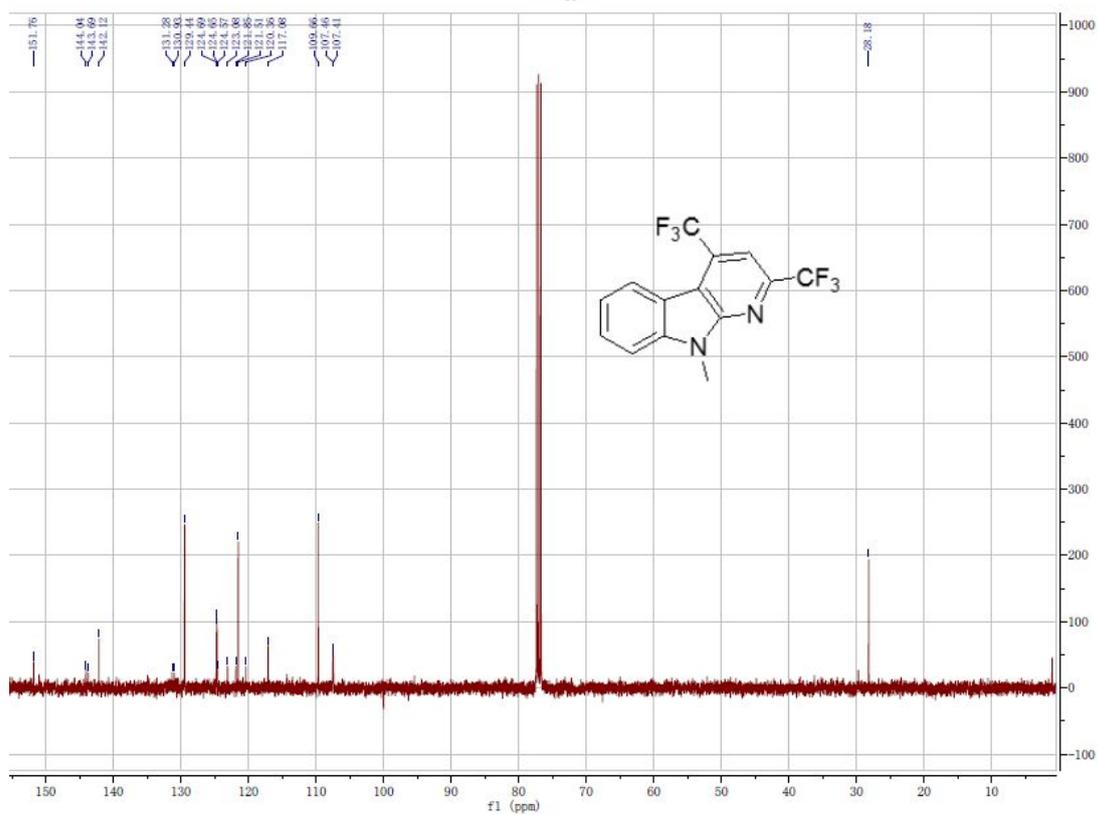
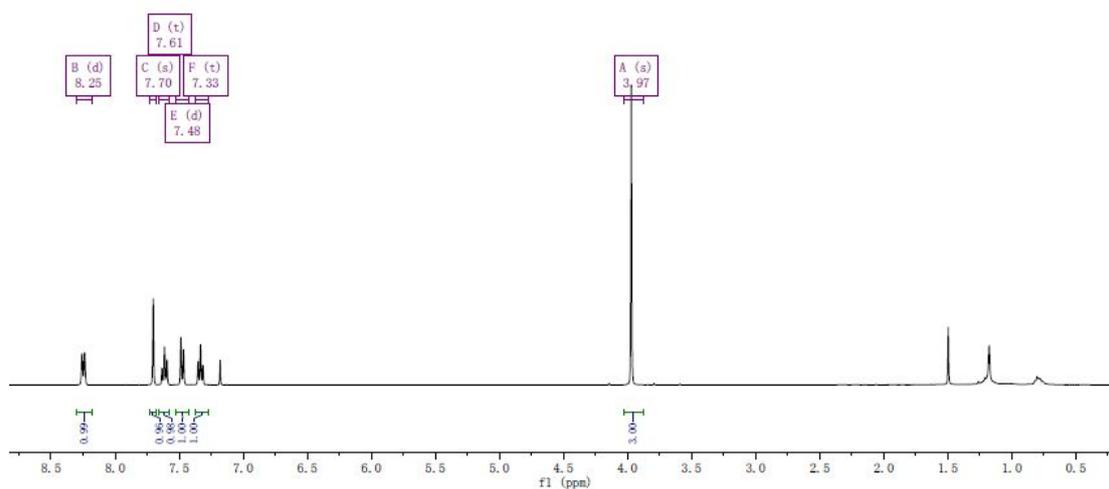
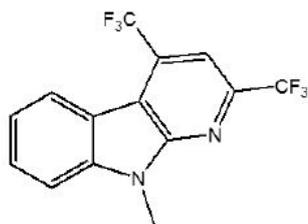
2,9-dimethyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3i)



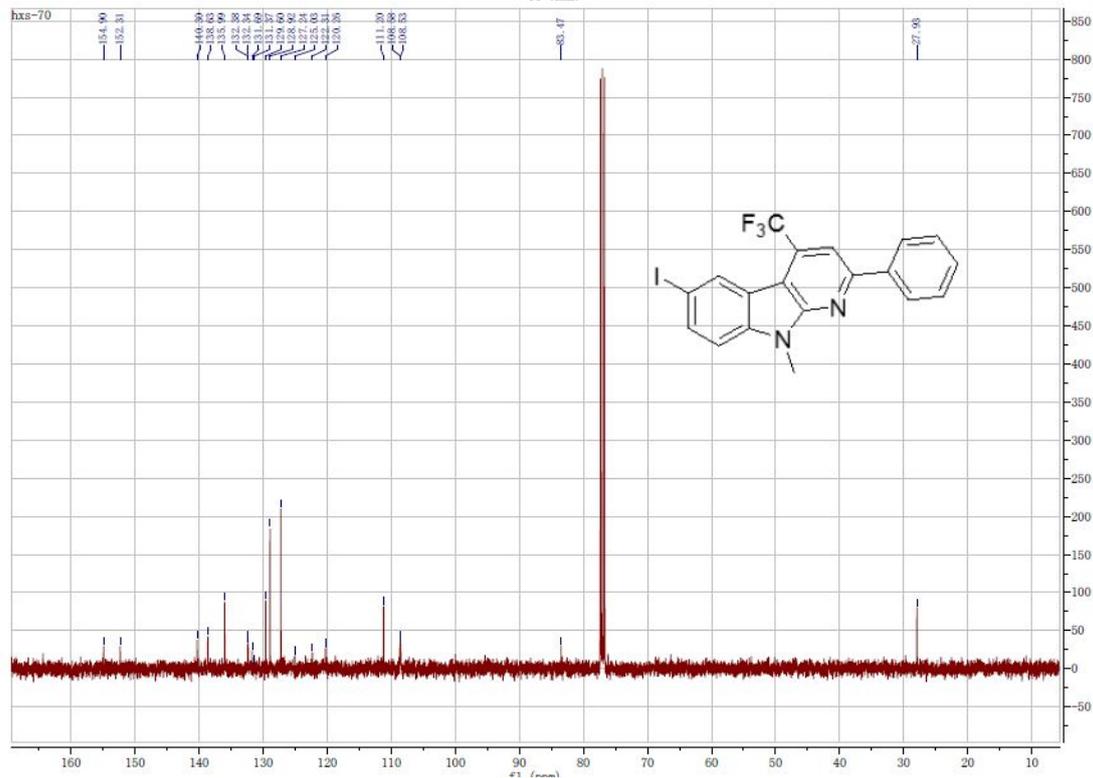
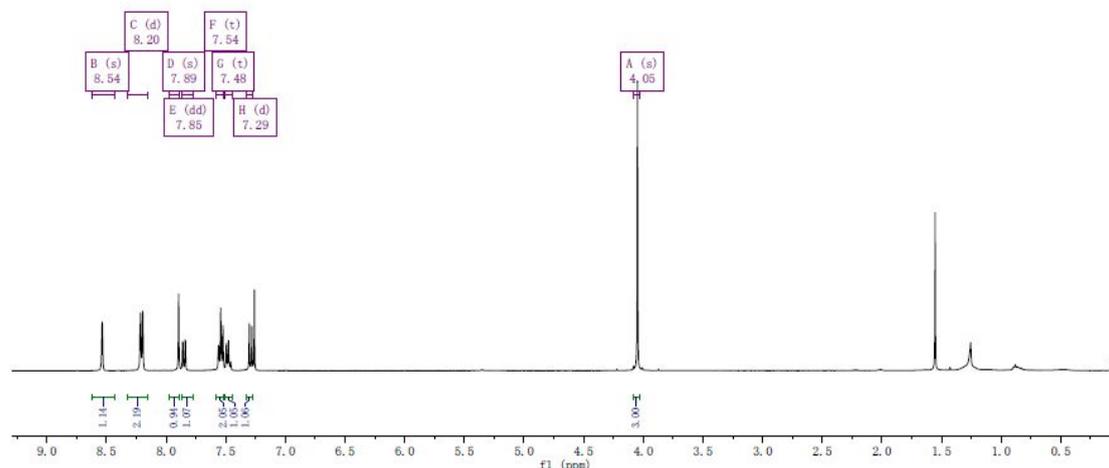
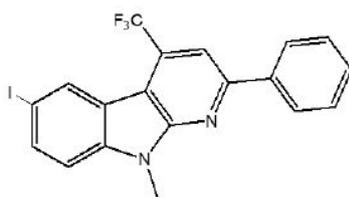
2,4,9-trimethyl-9H-pyrido[2,3-b]indole (3j)



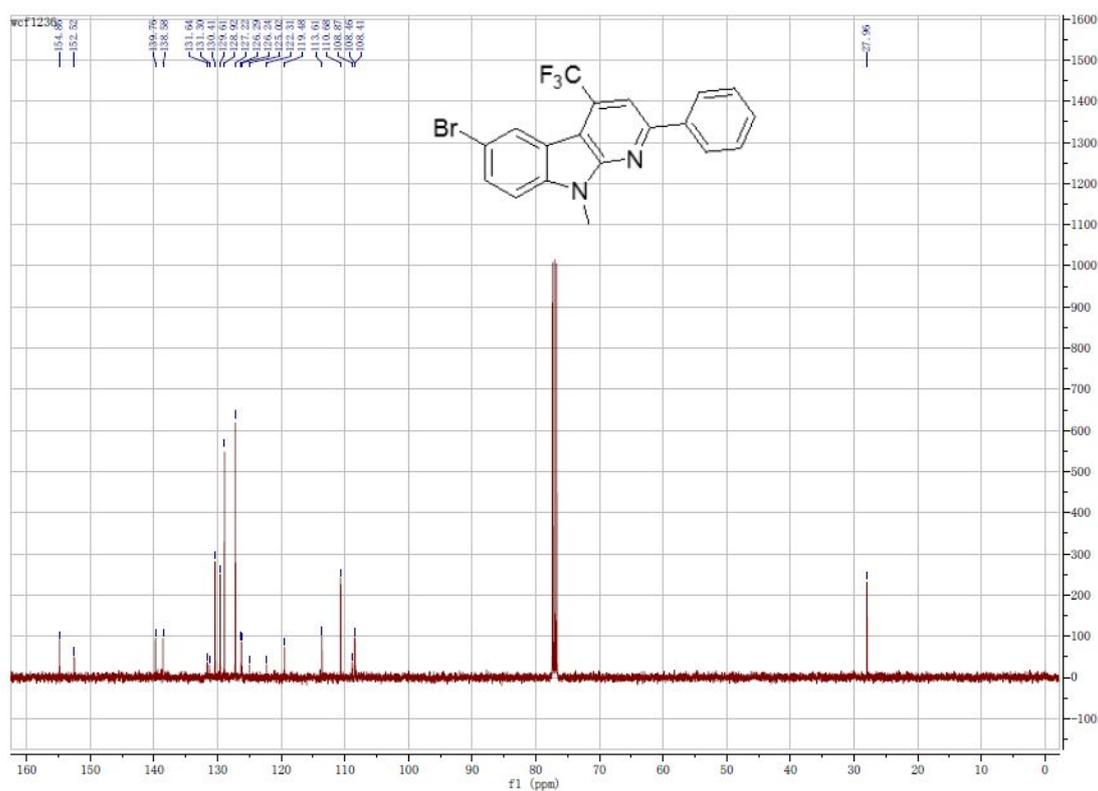
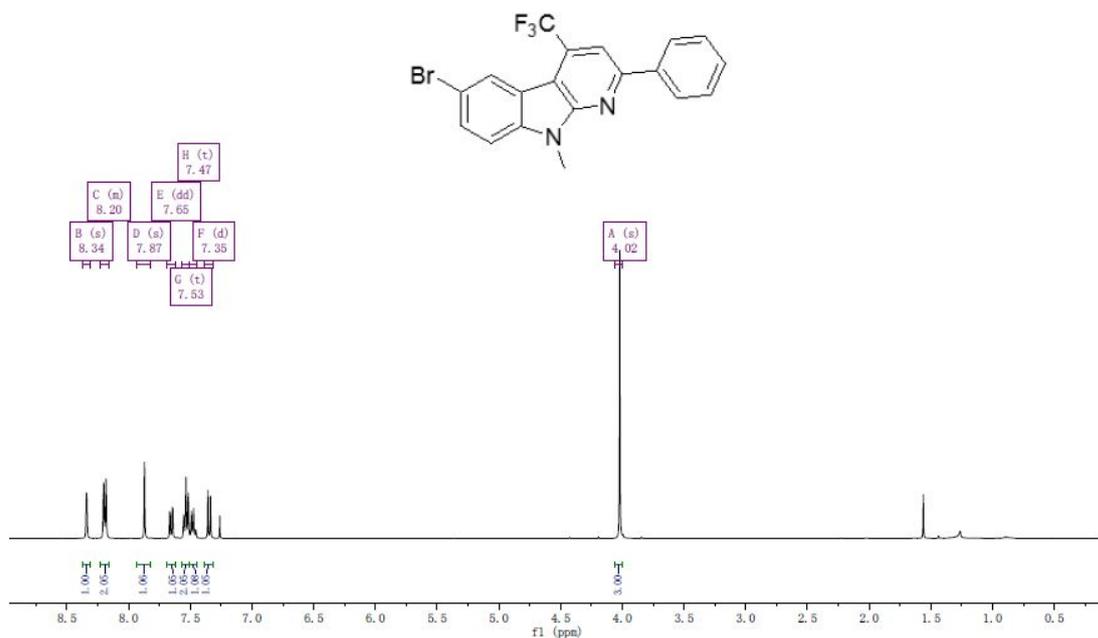
9-methyl-2,4-bis(trifluoromethyl)-9H-pyrido[2,3-b]indole (3k)



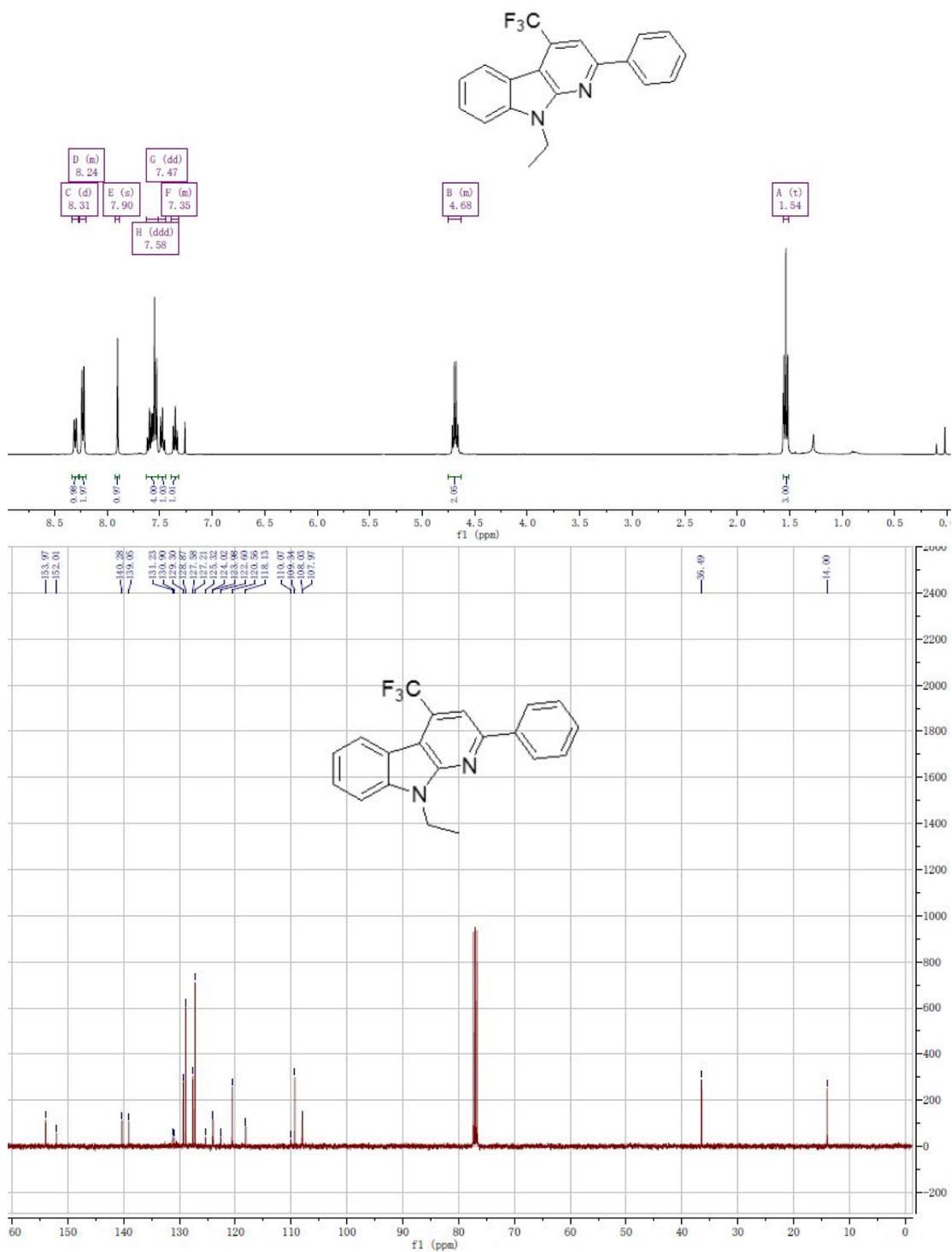
6-iodo-9-methyl-4-phenyl-2-(trifluoromethyl)-9H-pyrido[2,3-b]indole (31)



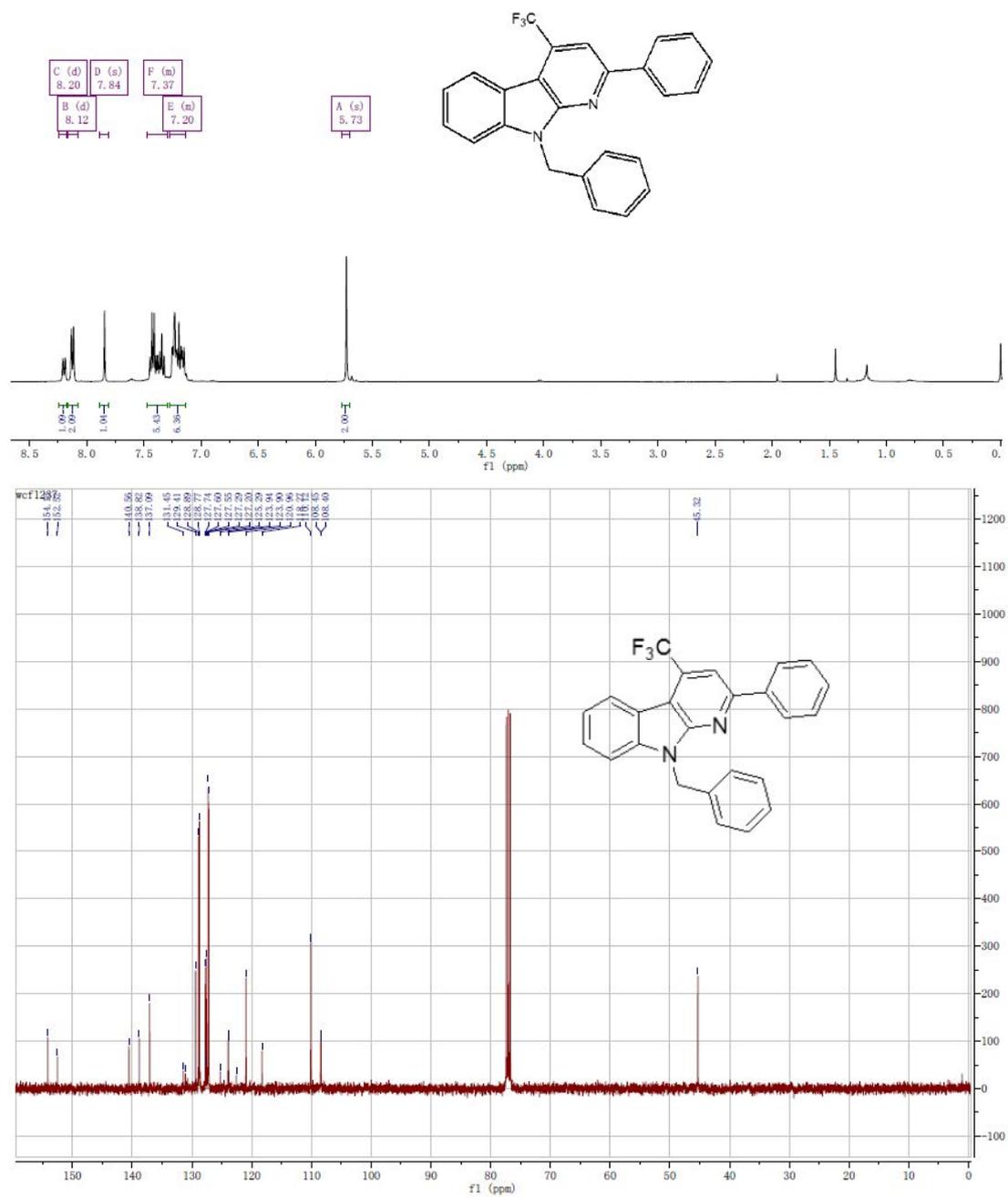
6-bromo-9-methyl-2-phenyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3m)



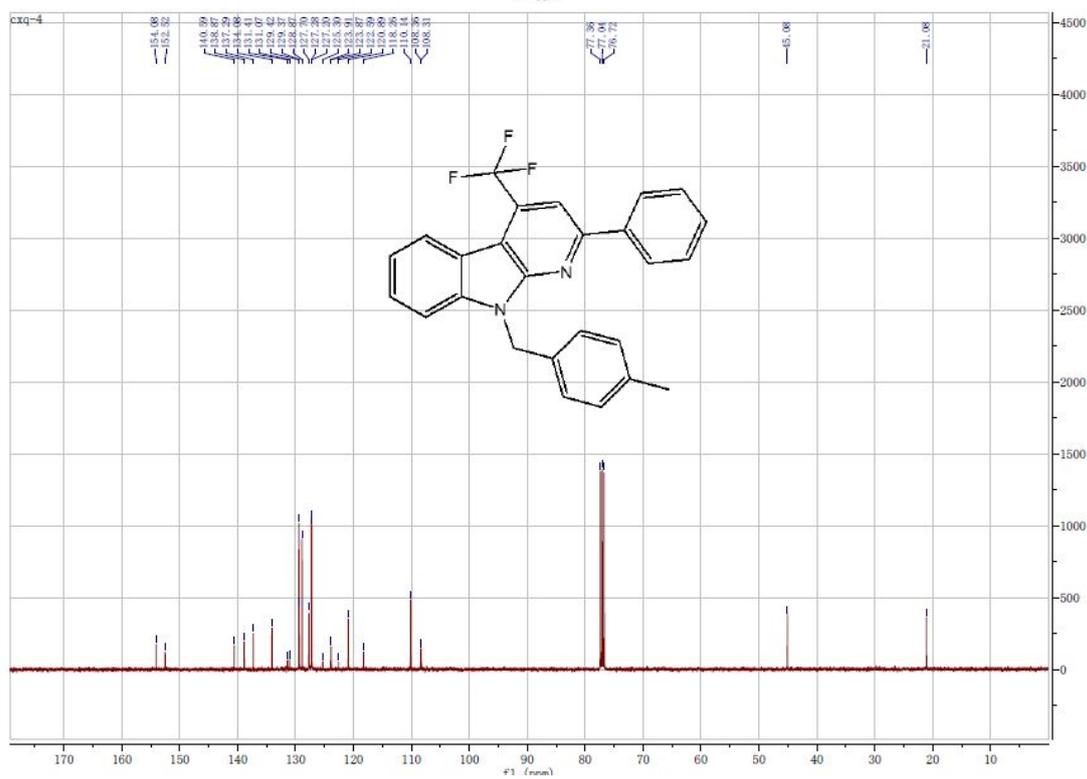
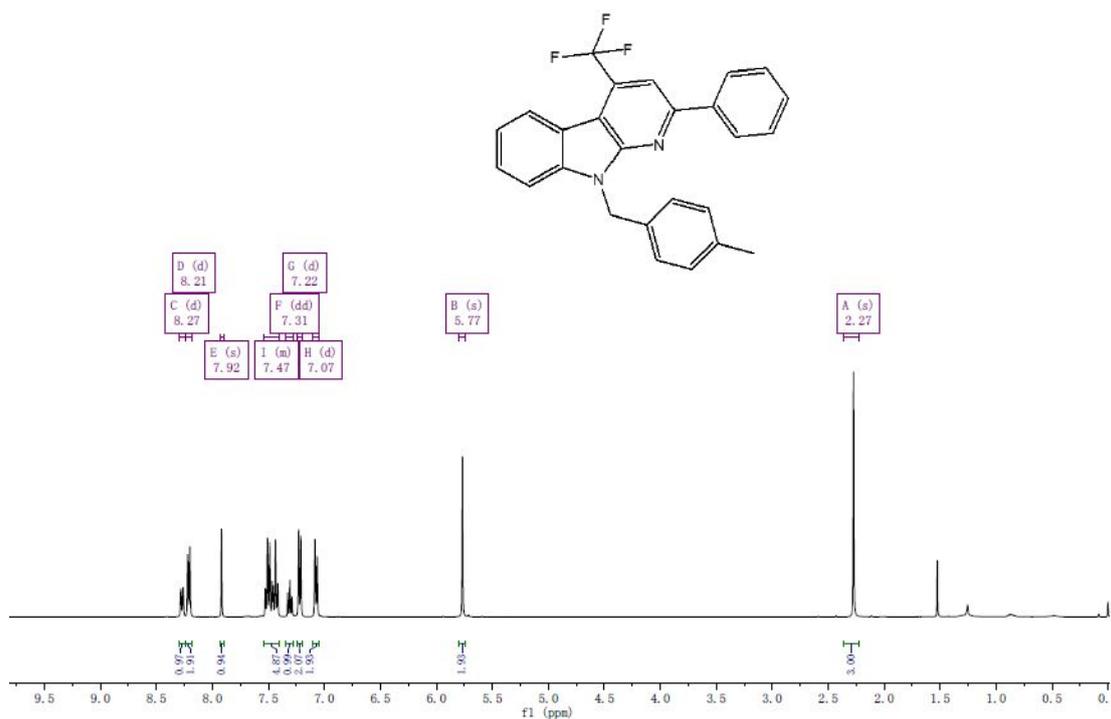
9-ethyl-2-phenyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3n)



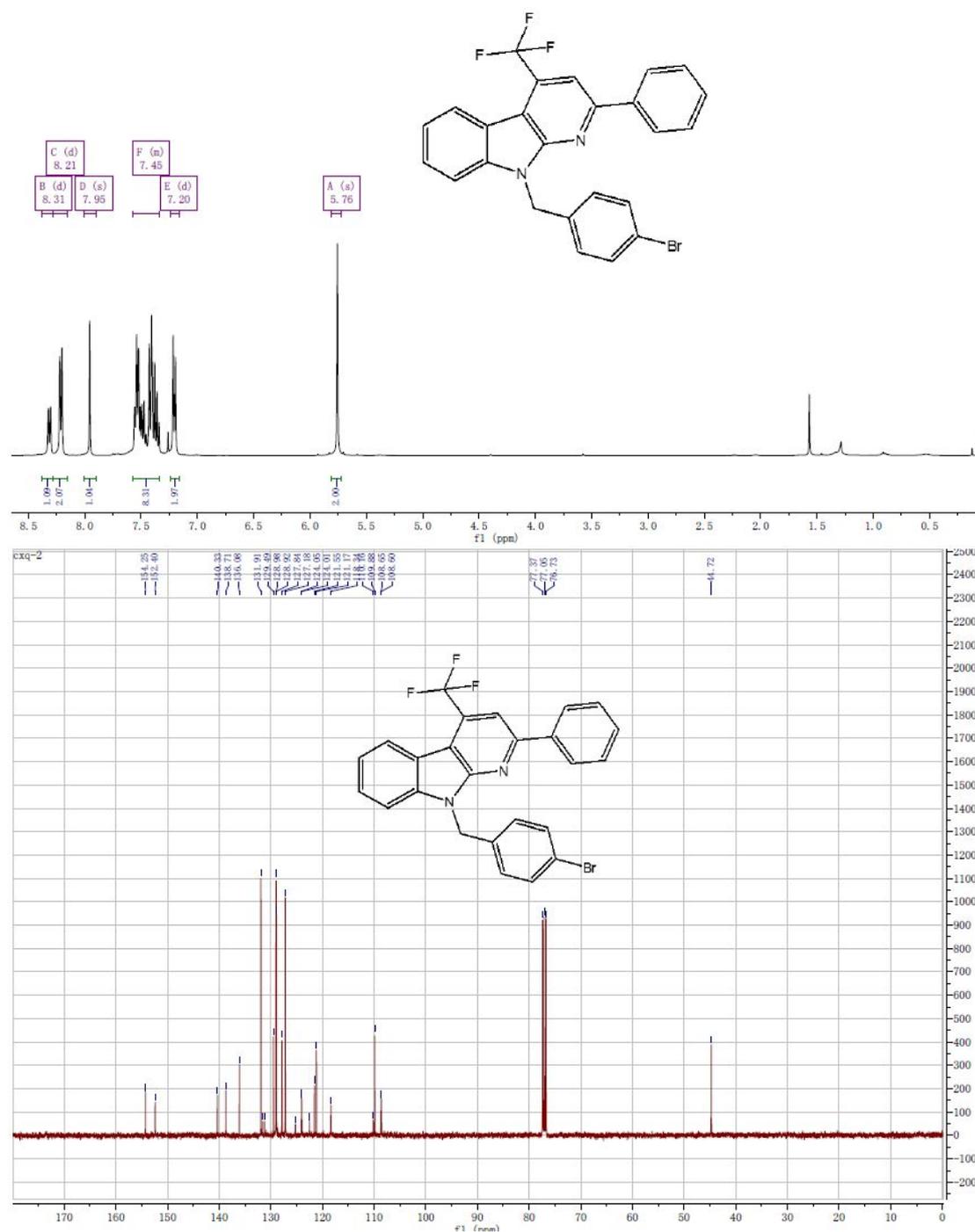
9-benzyl-2-phenyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3o)



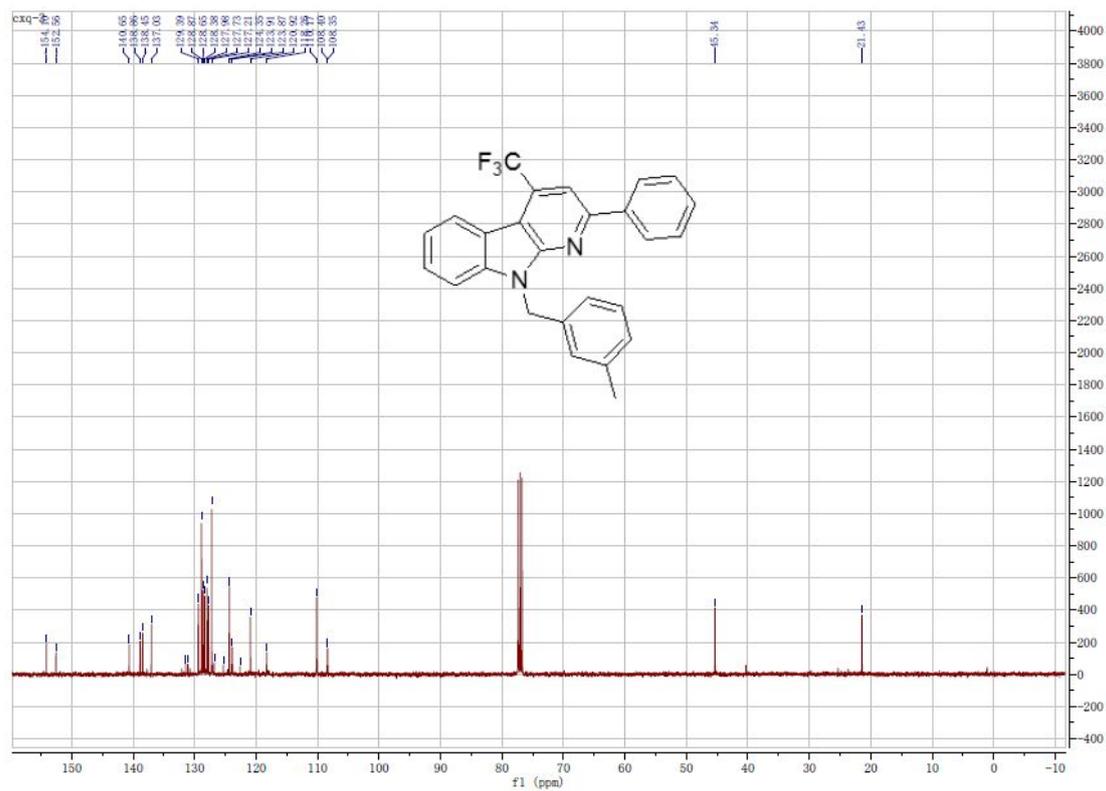
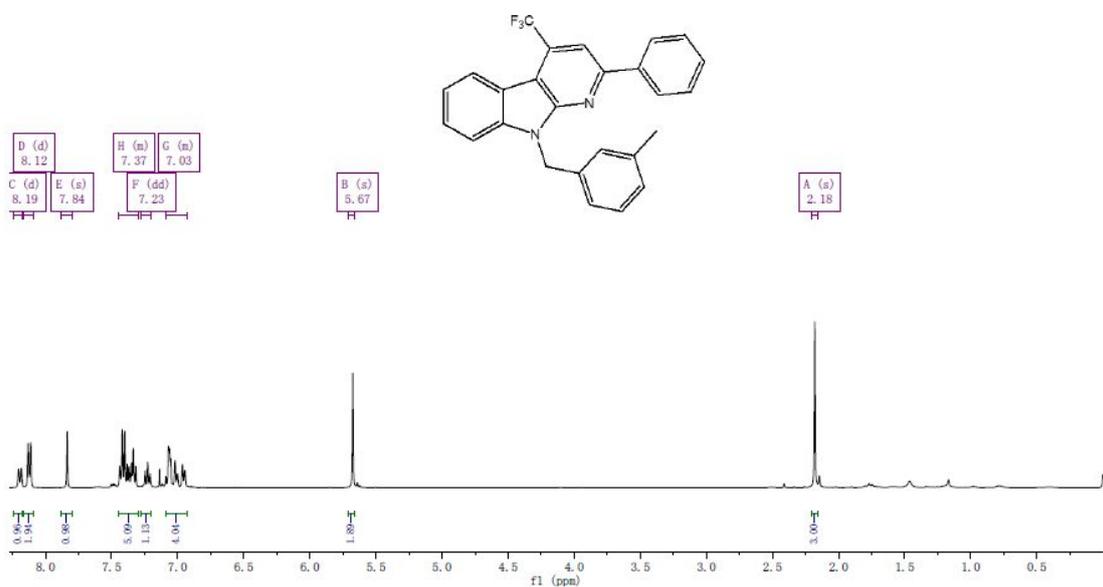
9-(4-methylbenzyl)-2-phenyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3q)



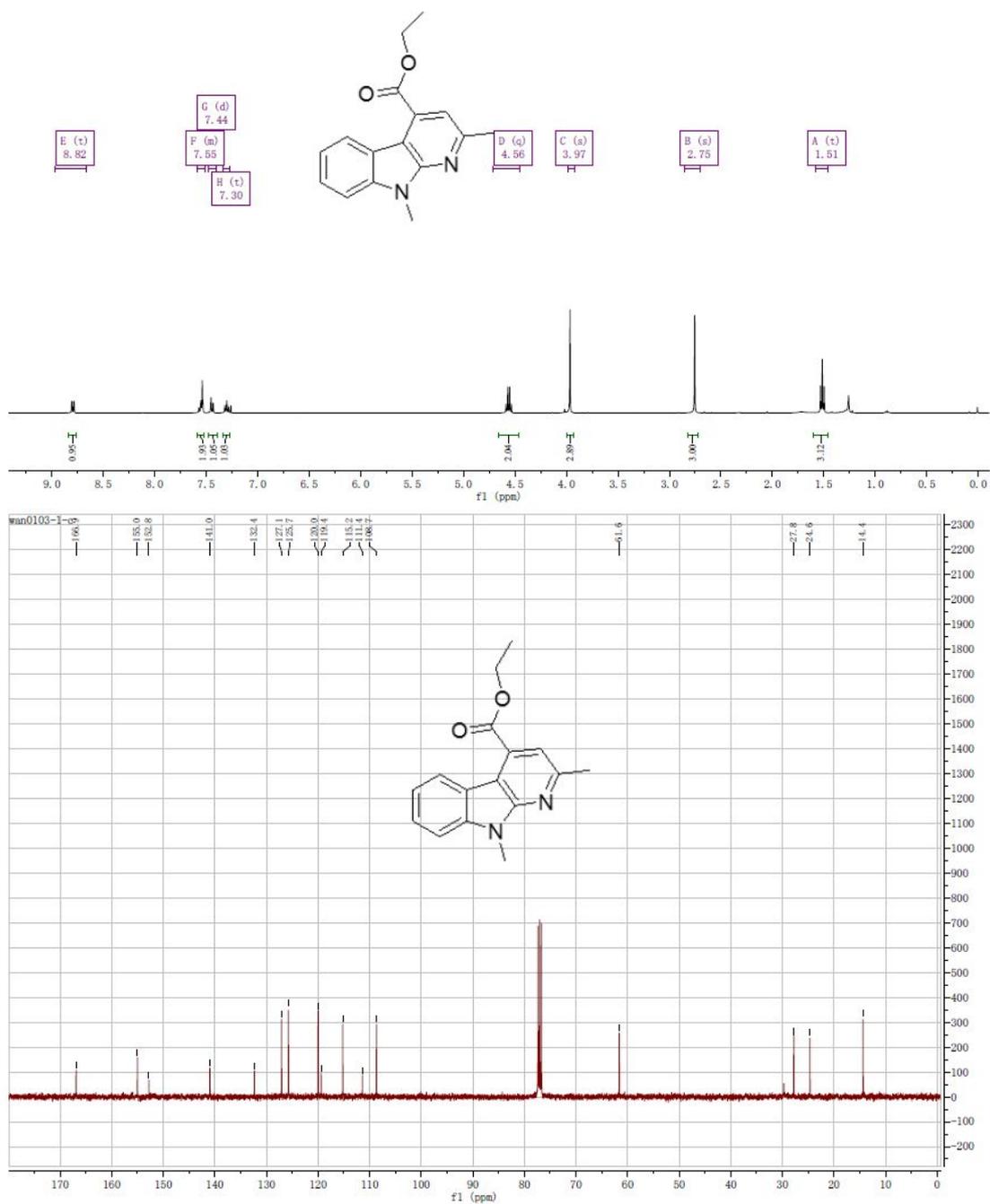
9-(4-bromo-2-phenyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3r)



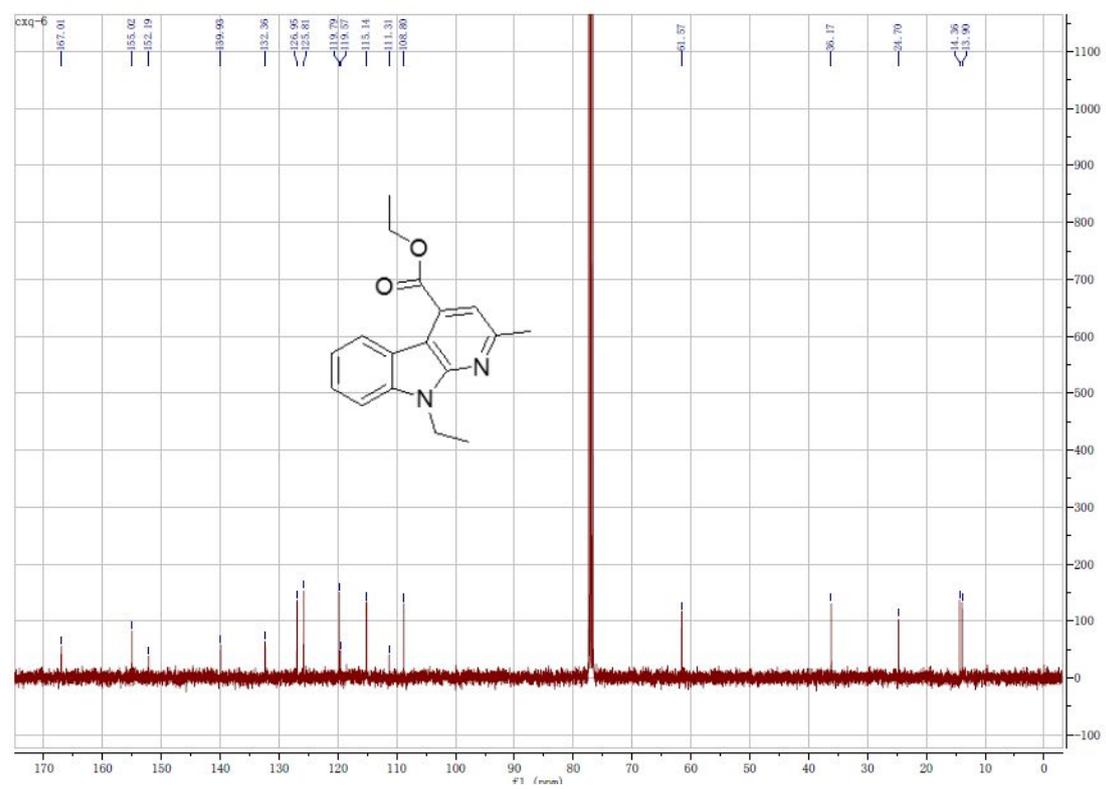
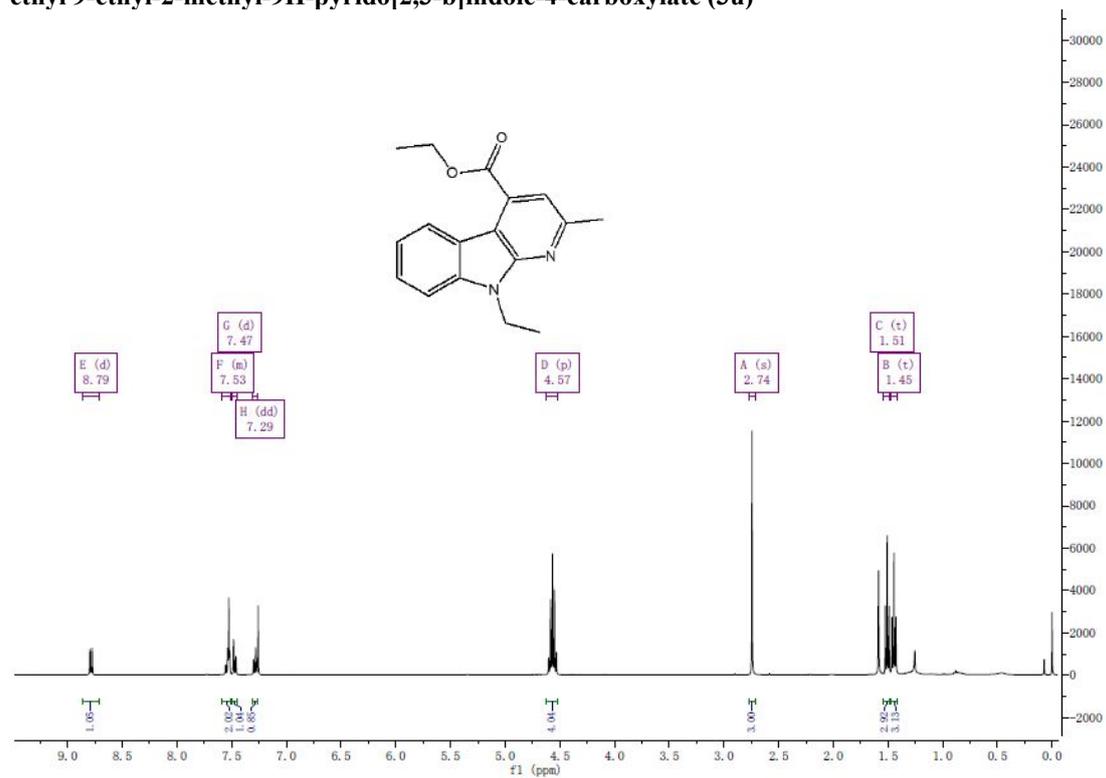
9-(3-methylbenzyl)-2-phenyl-4-(trifluoromethyl)-9H-pyrido[2,3-b]indole (3s)



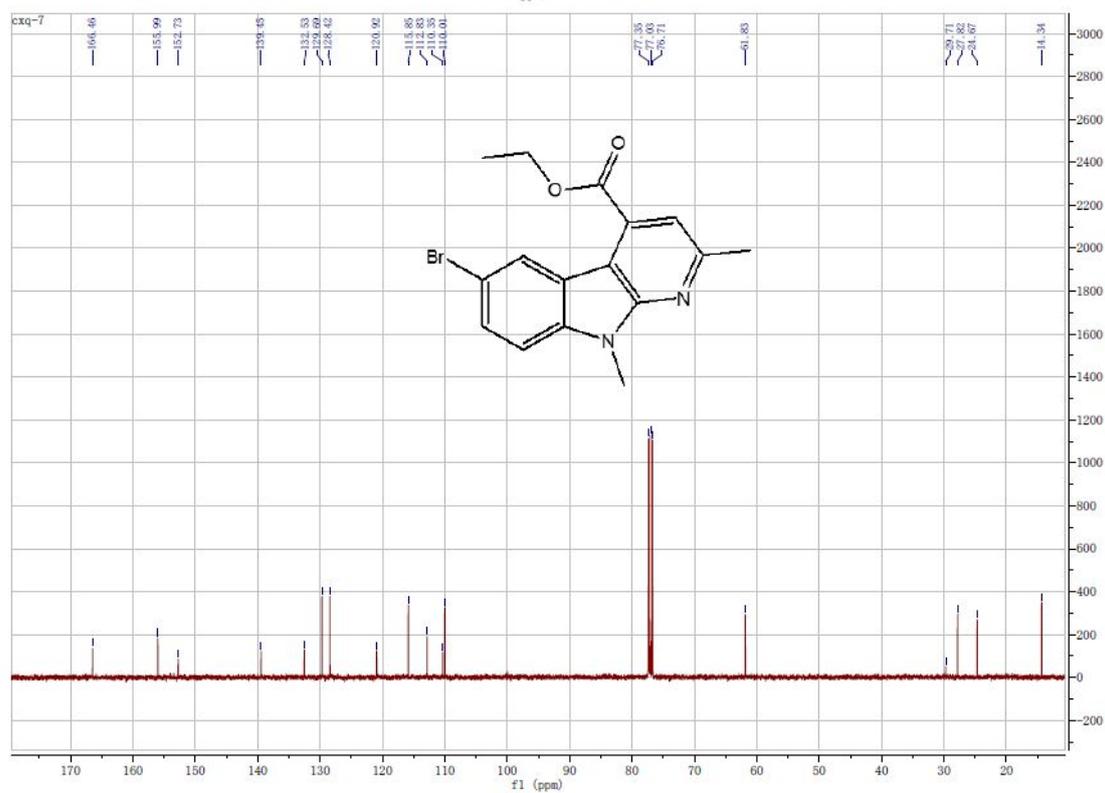
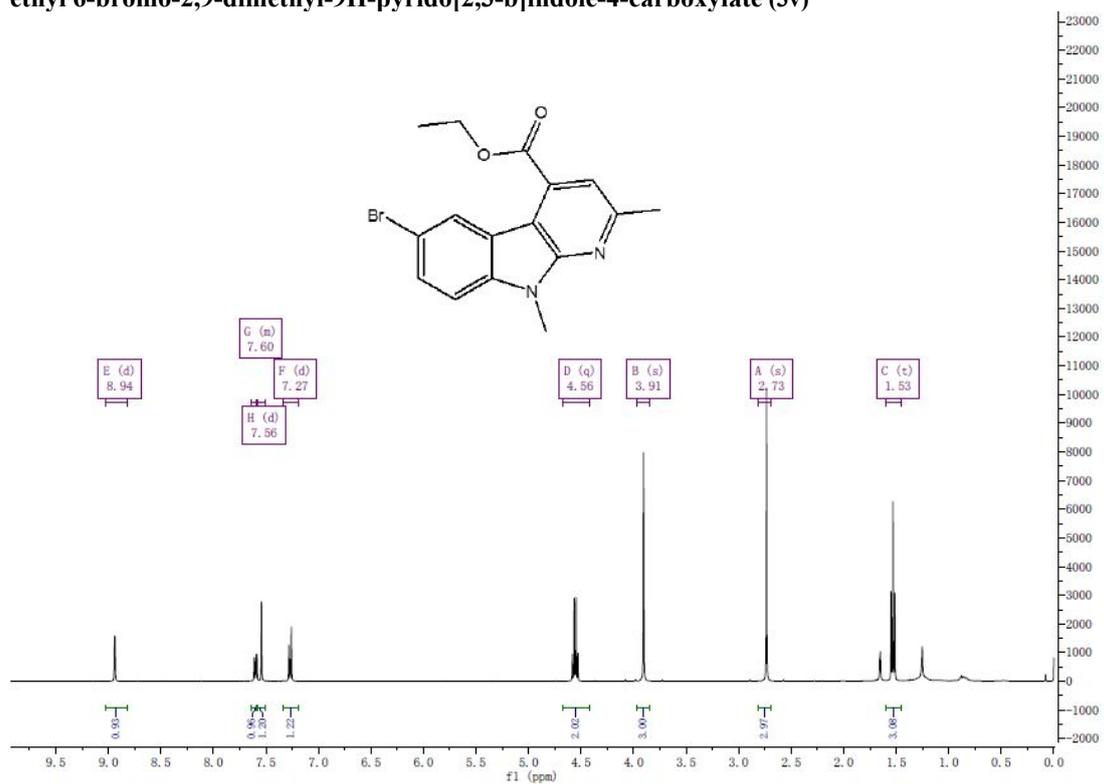
ethyl 2,9-dimethyl-9H-pyrido[2,3-b]indole-4-carboxylate (3t)



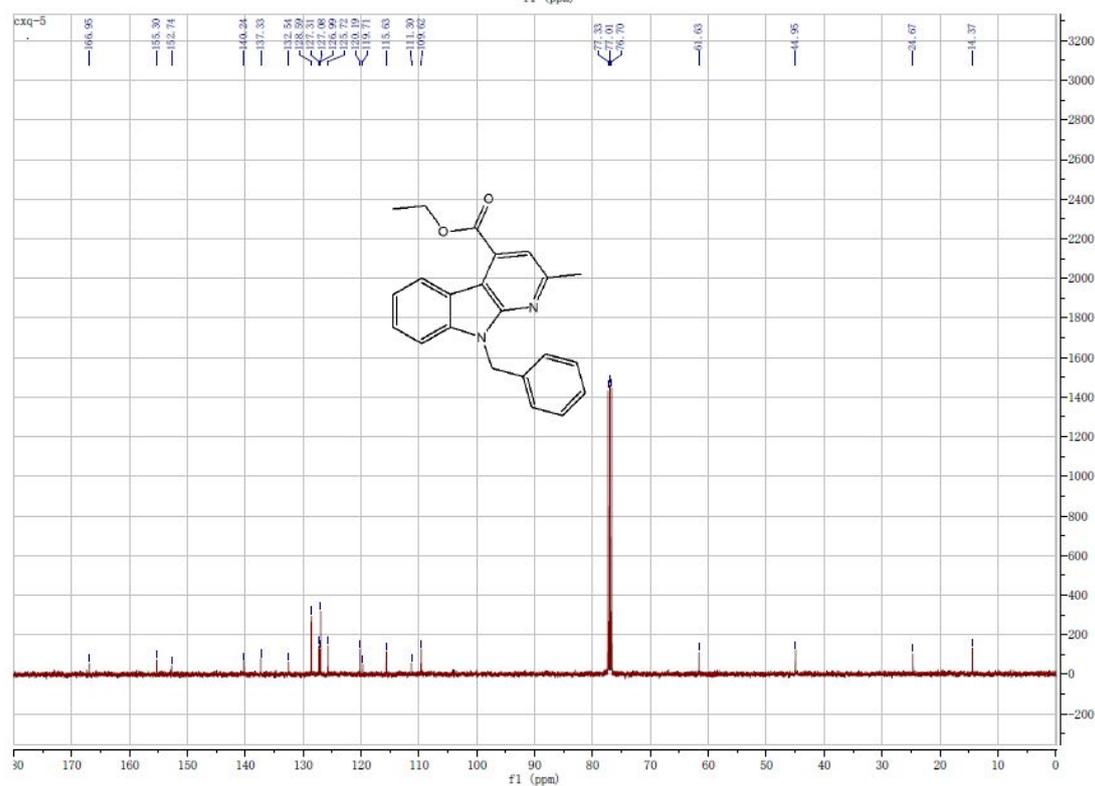
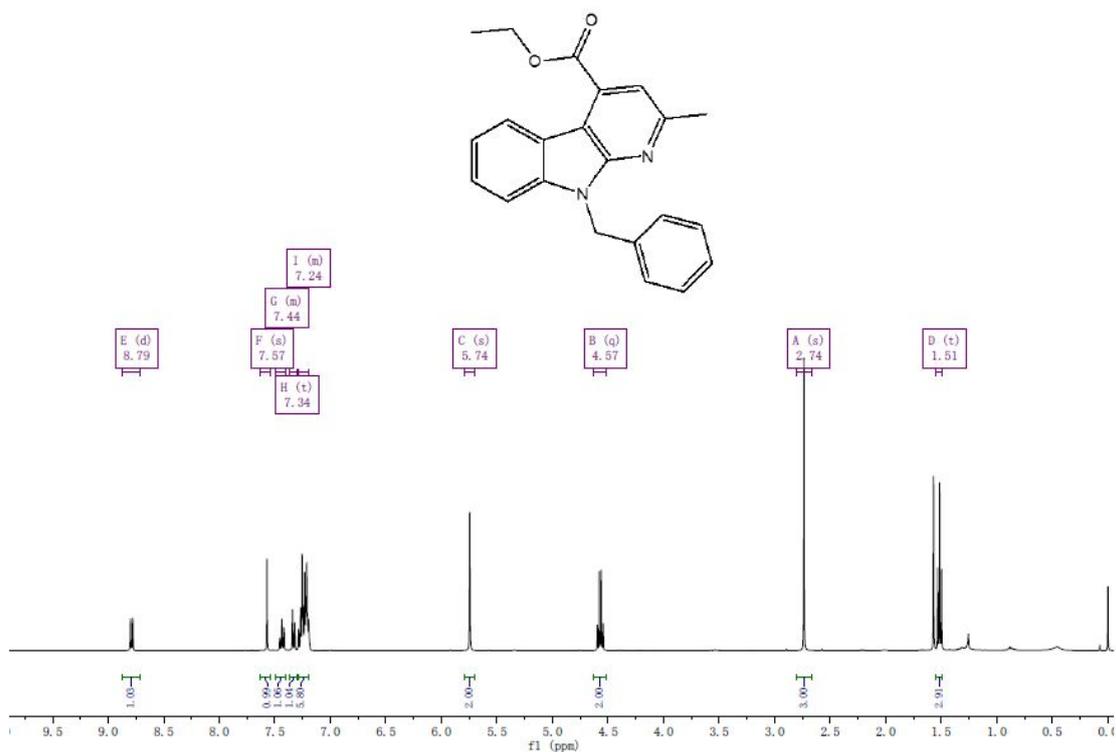
ethyl 9-ethyl-2-methyl-9H-pyrido[2,3-b]indole-4-carboxylate (3u)



ethyl 6-bromo-2,9-dimethyl-9H-pyrido[2,3-b]indole-4-carboxylate (3v)

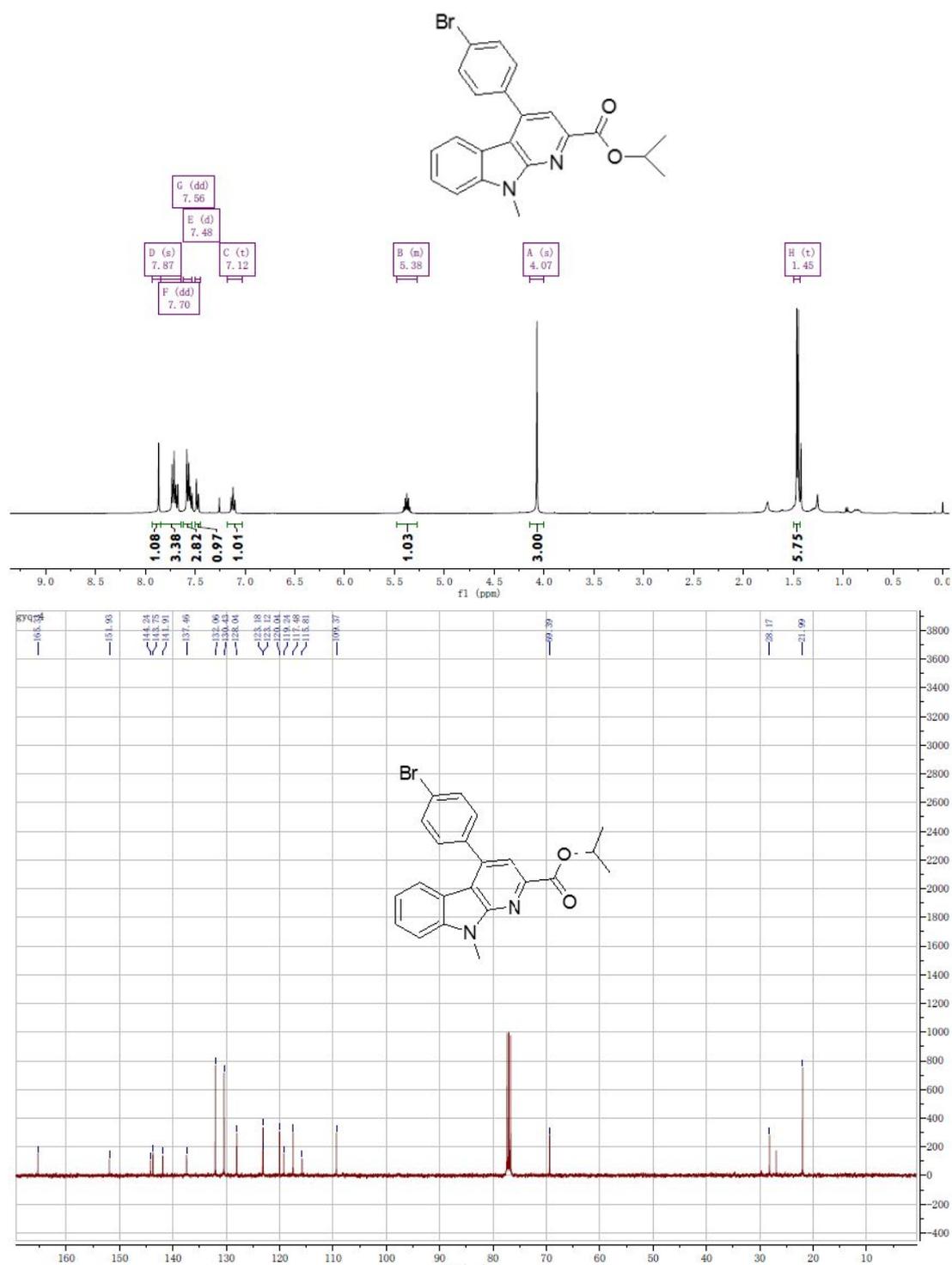


ethyl 9-benzyl-2-methyl-9H-pyrido[2,3-b]indole-4-carboxylate (3w)

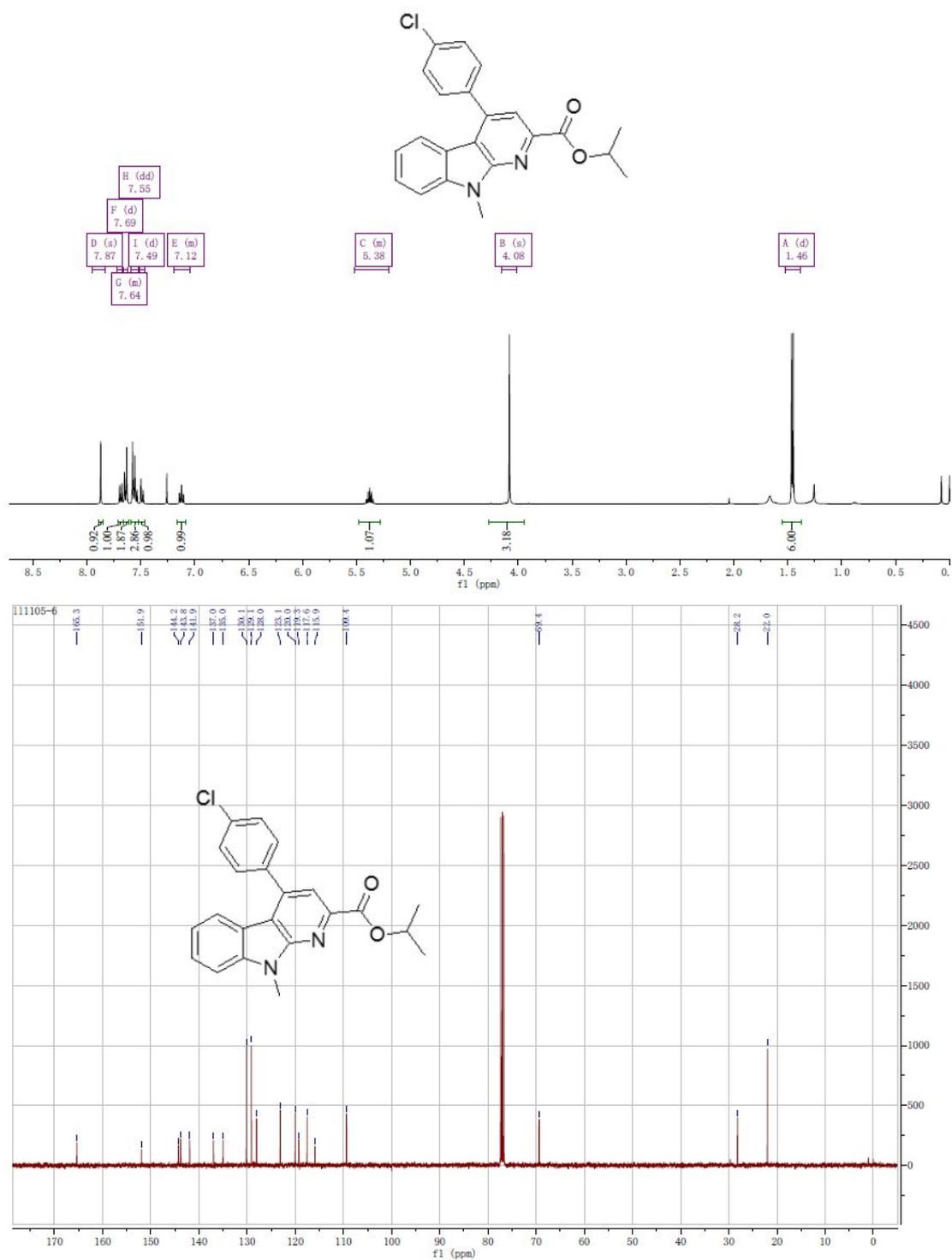


isopropyl 4-(4-bromophenyl)-9-methyl-9H-pyrido[2,3-b]indole-2-carboxylate (5a)

879-4

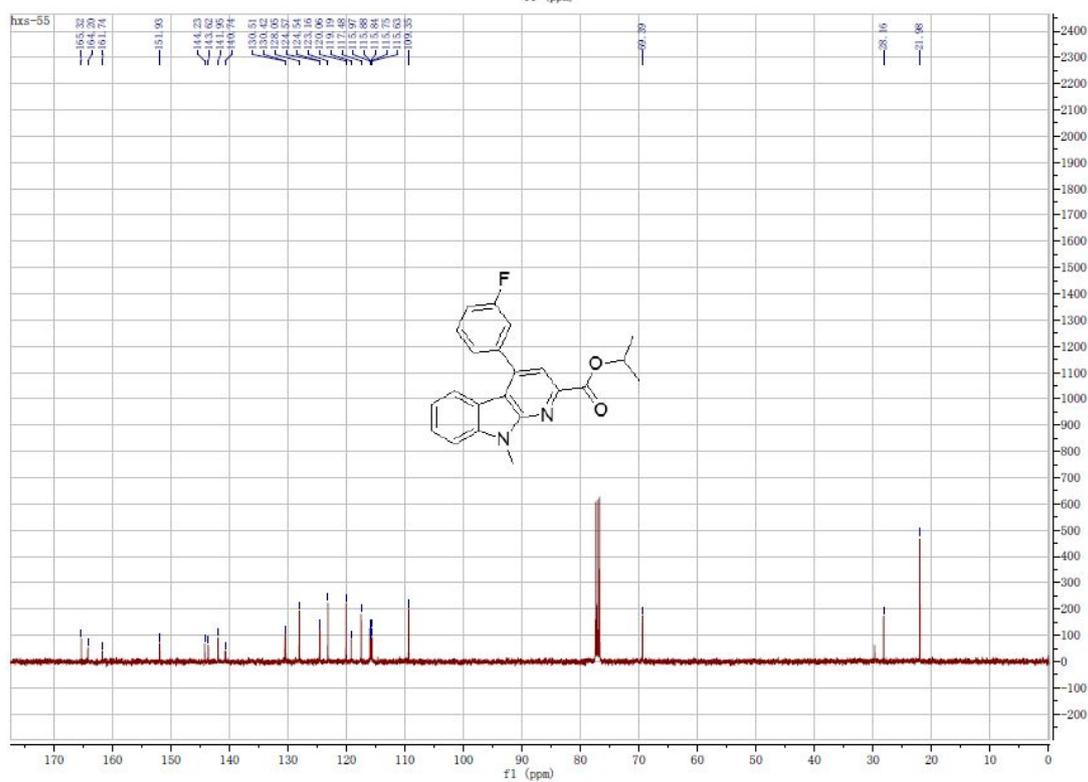
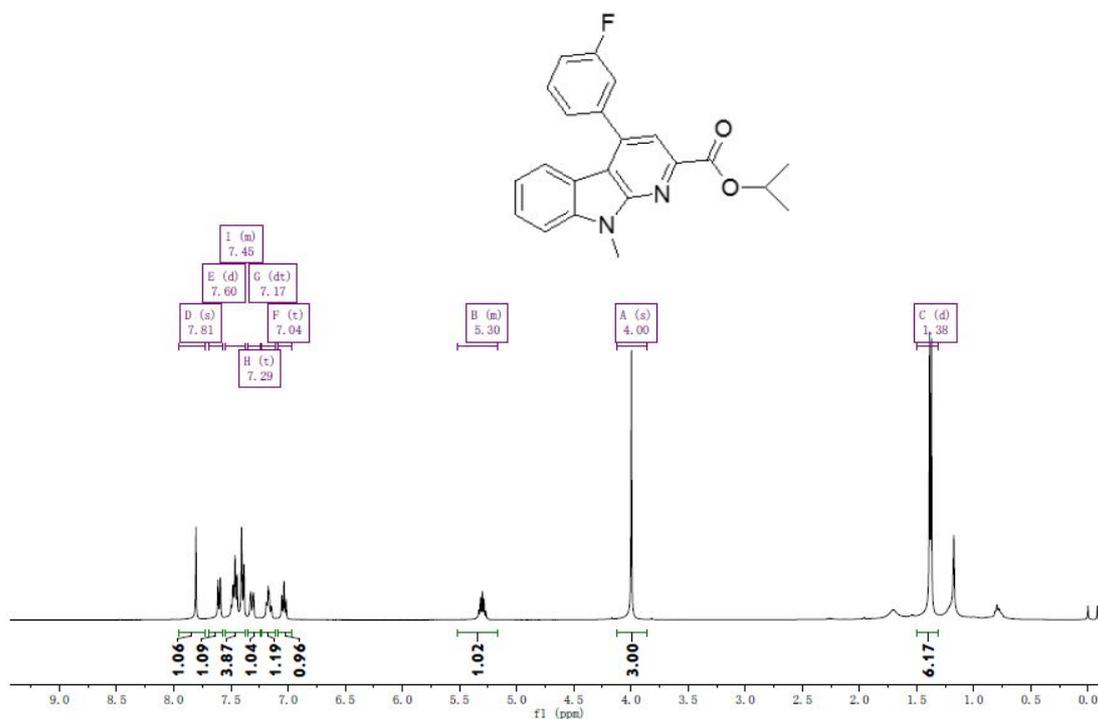


isopropyl 4-(4-chlorophenyl)-9-methyl-9H-pyrido[2,3-b]indole-2-carboxylate (5b)

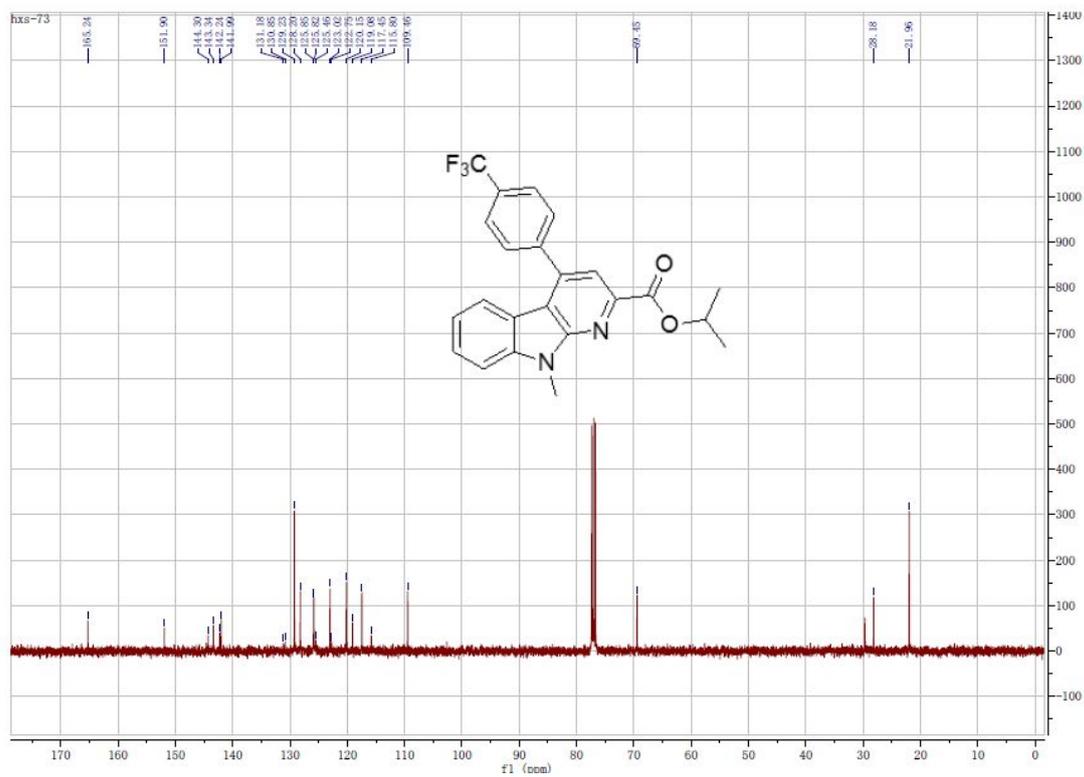
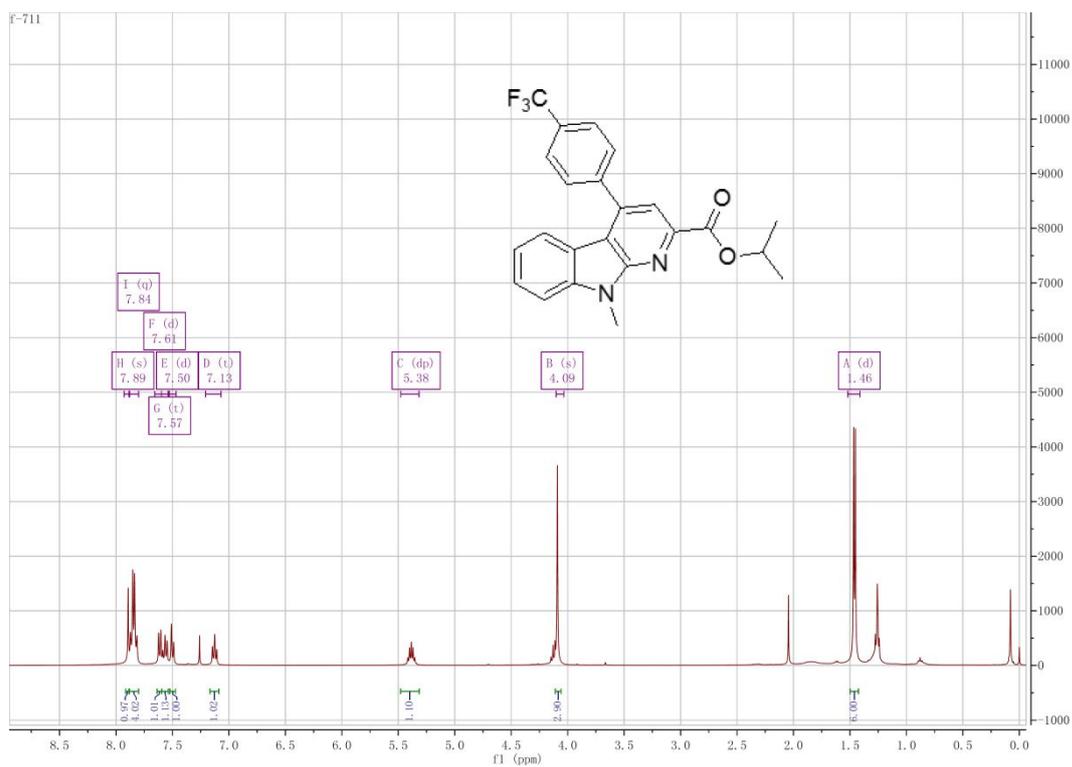


isopropyl 4-(3-fluorophenyl)-9-methyl-9H-pyrido[2,3-b]indole-2-carboxylate (5c)

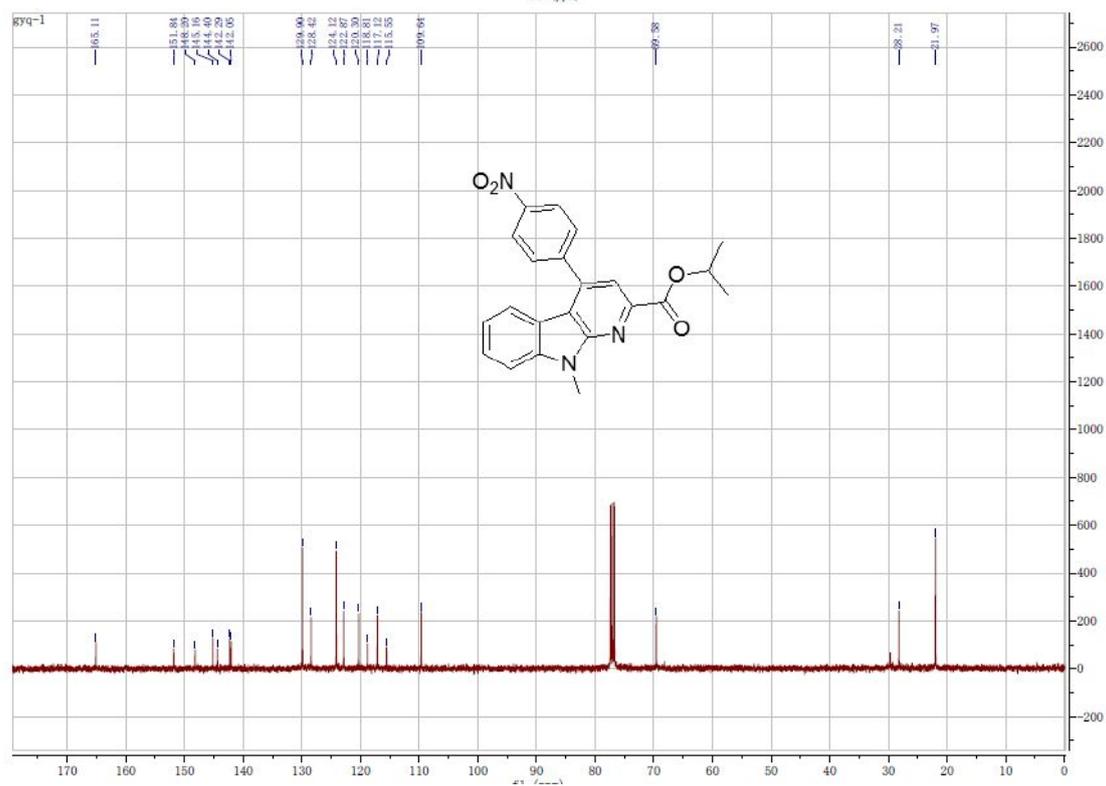
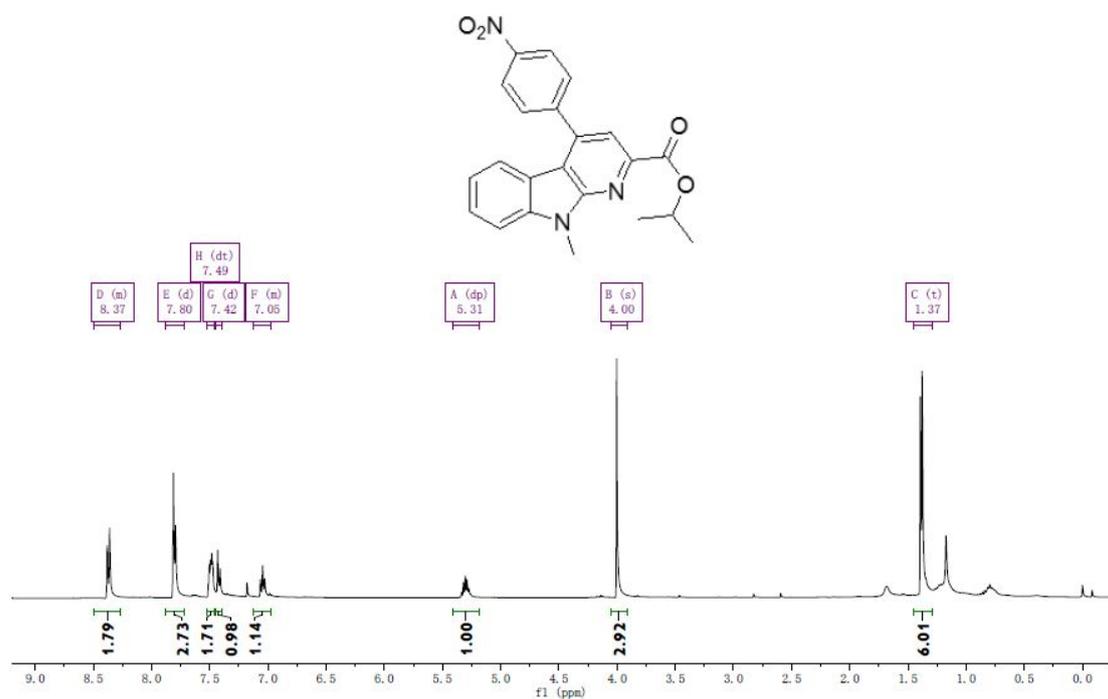
hxs-55



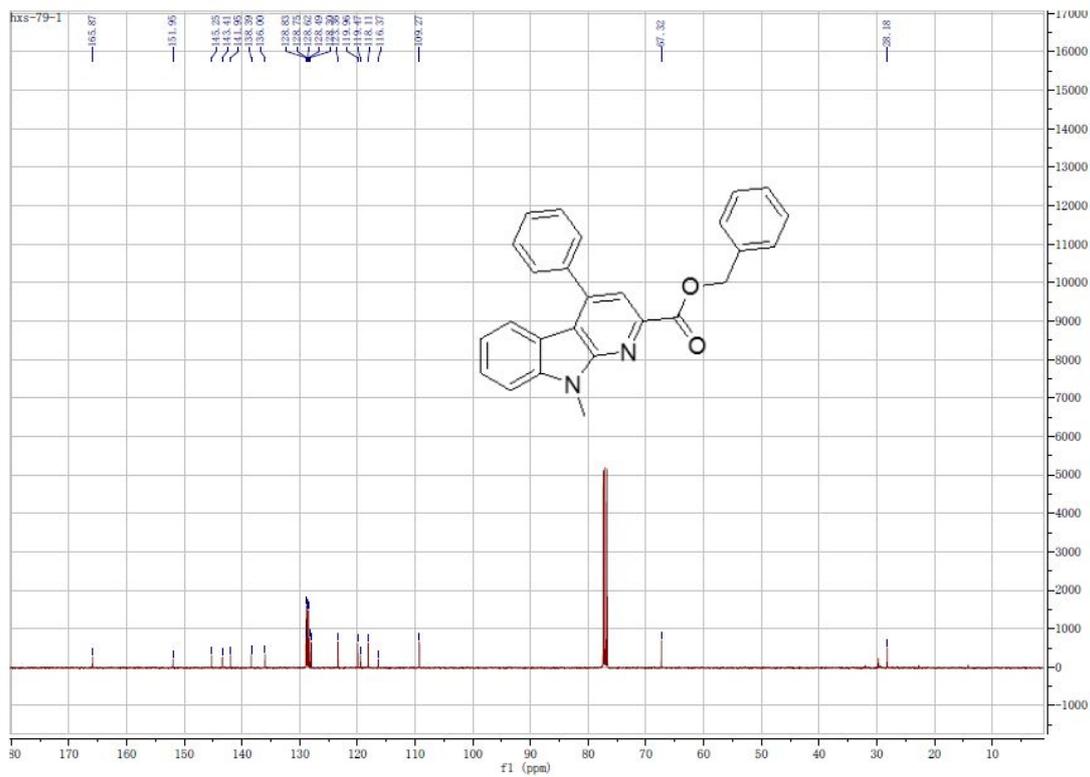
isopropyl 9-methyl-4-(4-(trifluoromethyl)phenyl)-9H-pyrido[2,3-b]indole-2-carboxylate (5d)



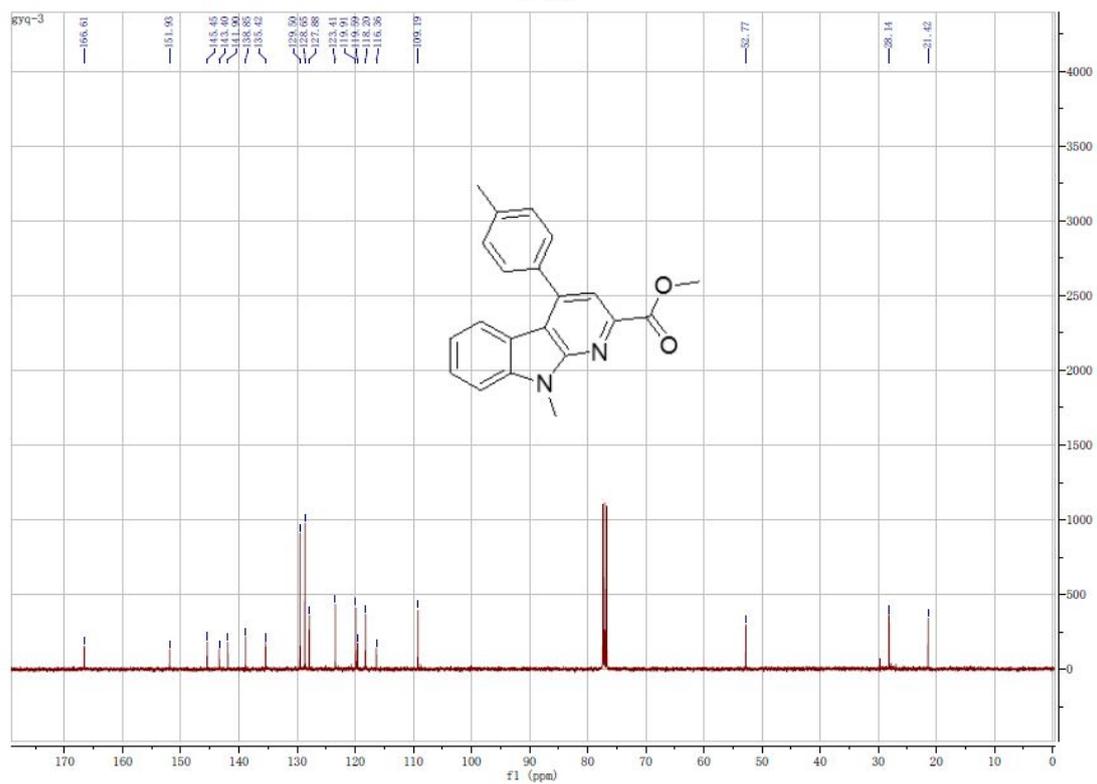
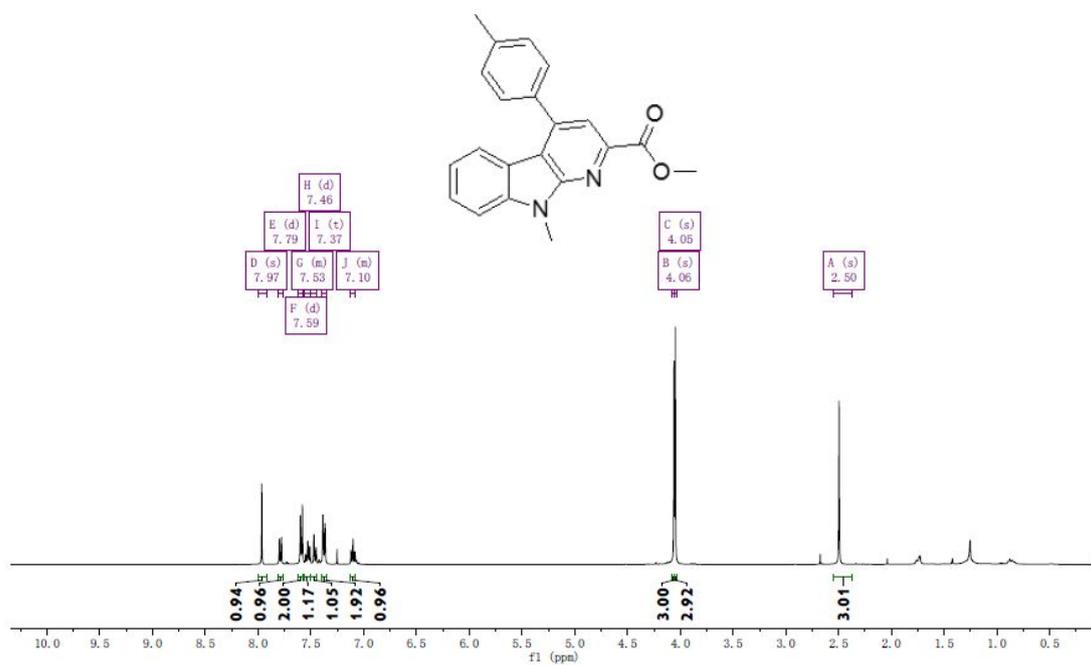
isopropyl 9-methyl-4-(4-nitrophenyl)-9H-pyrido[2,3-b]indole-2-carboxylate (5e)



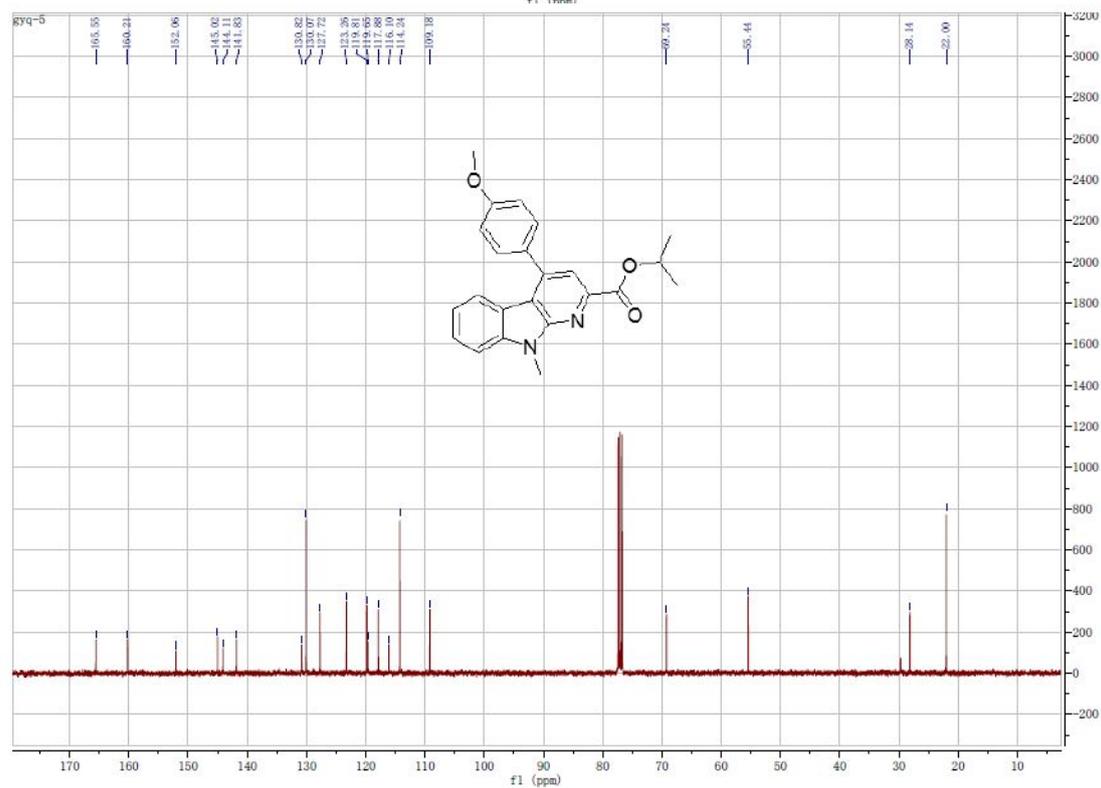
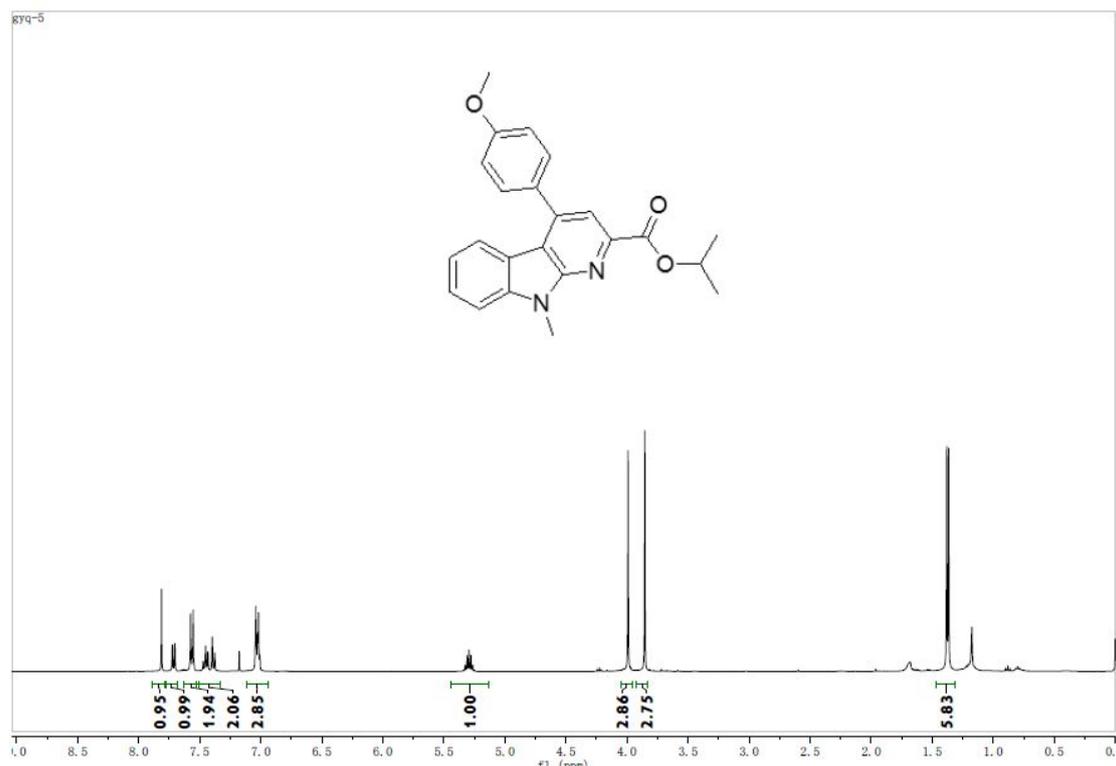
benzyl 9-methyl-4-phenyl-9H-pyrido[2,3-b]indole-2-carboxylate (5f)



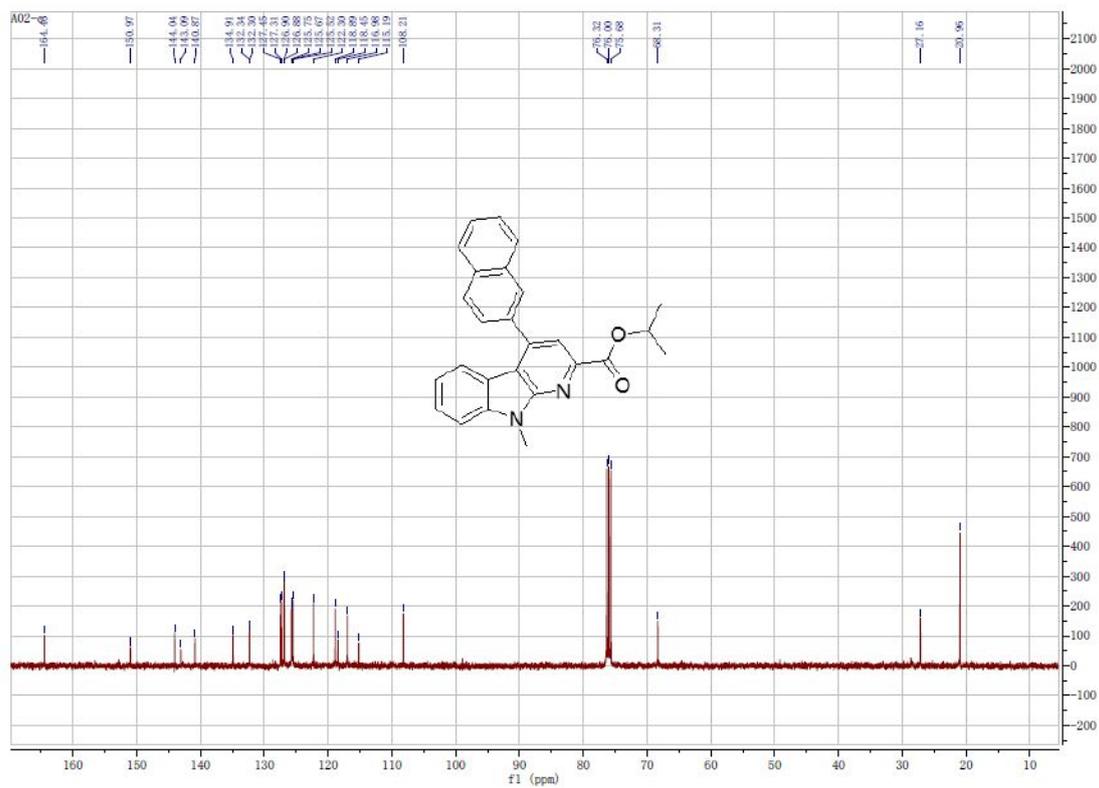
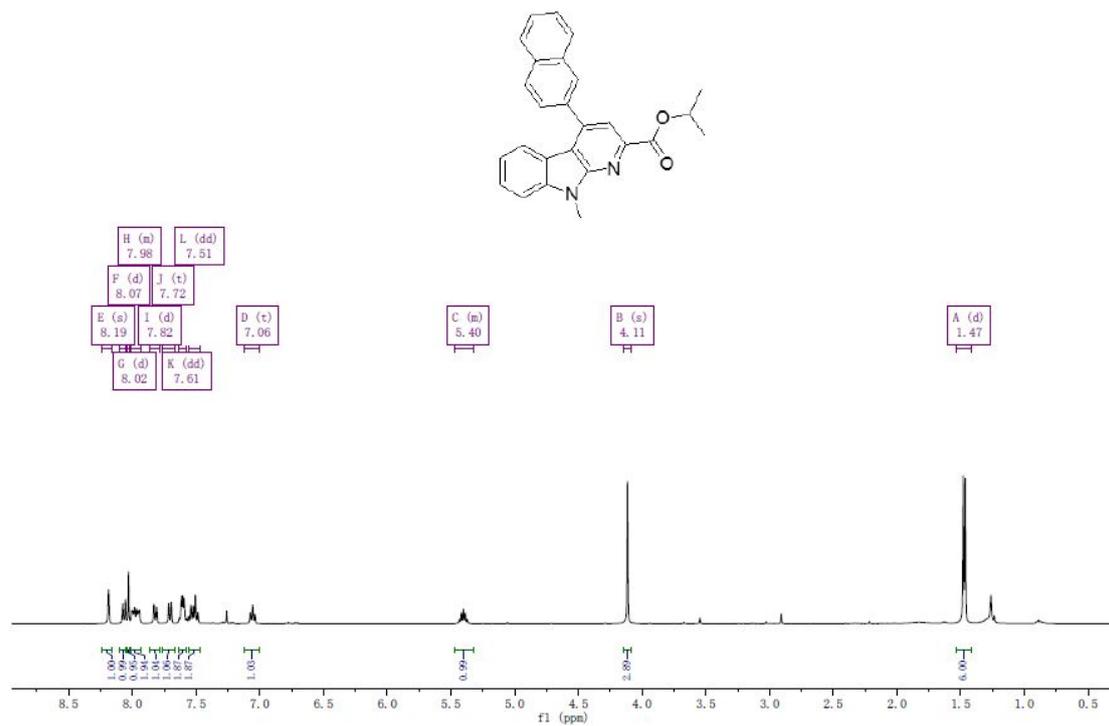
methyl 9-methyl-4-p-tolyl-9H-pyrido[2,3-b]indole-2-carboxylate (5g)



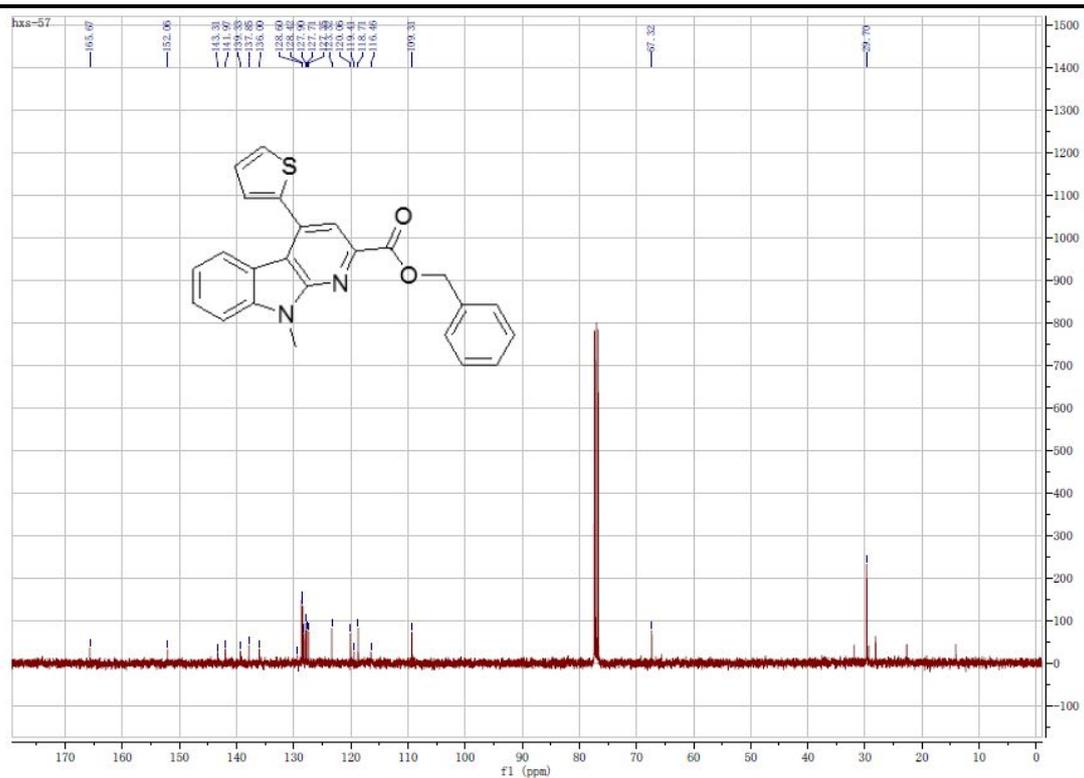
isopropyl 4-(4-methoxyphenyl)-9-methyl-9H-pyrido[2,3-b]indole-2-carboxylate (5h)



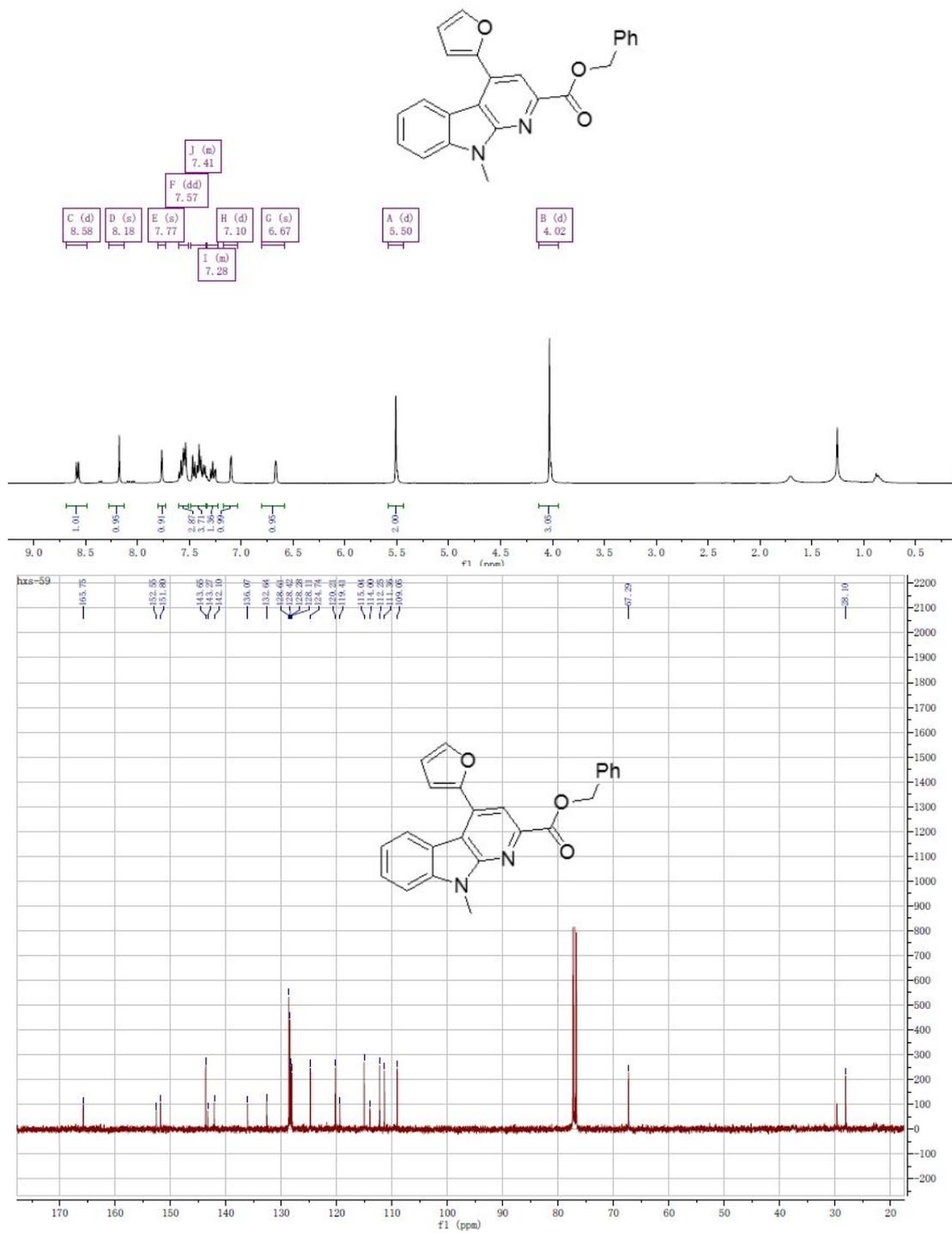
isobutyl 9-methyl-4-(naphthalen-2-yl)-9H-pyrido[2,3-b]indole-2-carboxylate (5i)



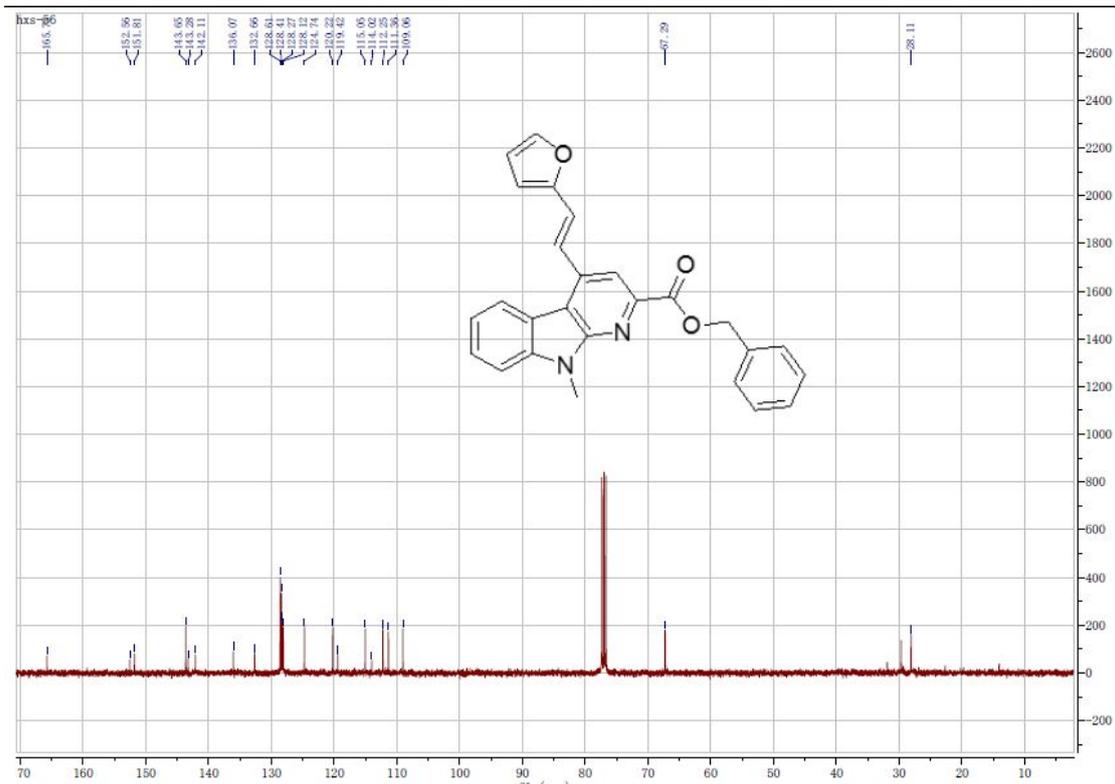
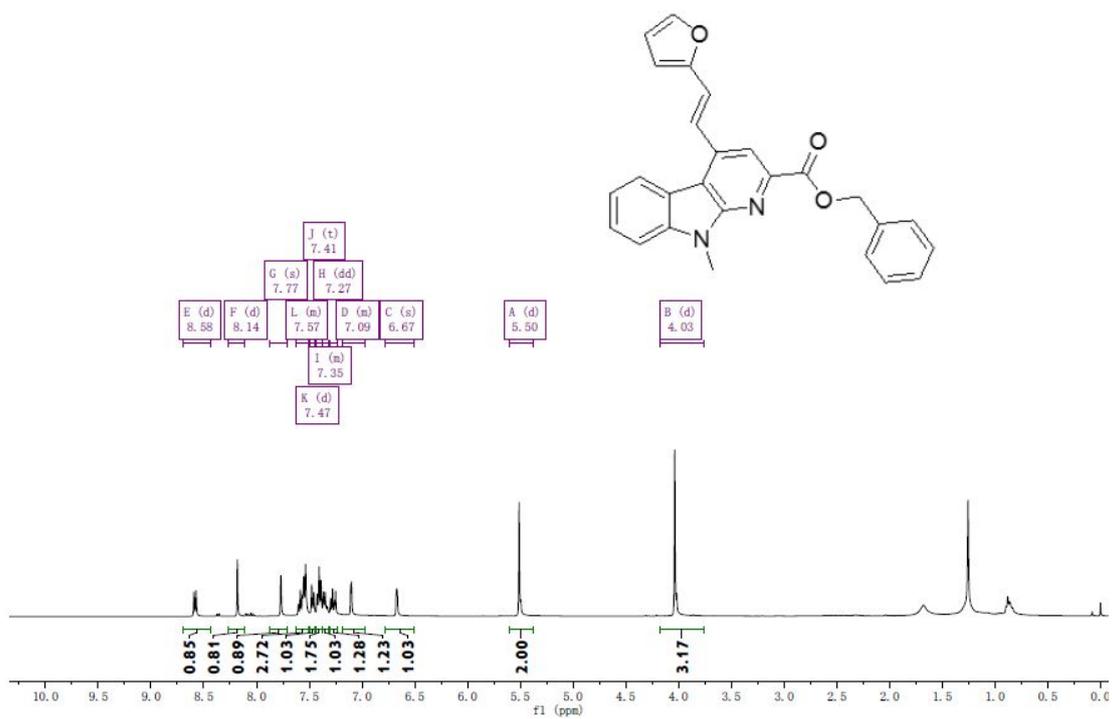
benzyl 9-methyl-4-(thiophen-2-yl)-9H-pyrido[2,3-b]indole-2-carboxylate (5j)



benzyl 4-(furan-2-yl)-9-methyl-9H-pyrido[2,3-b]indole-2-carboxylate (5k)



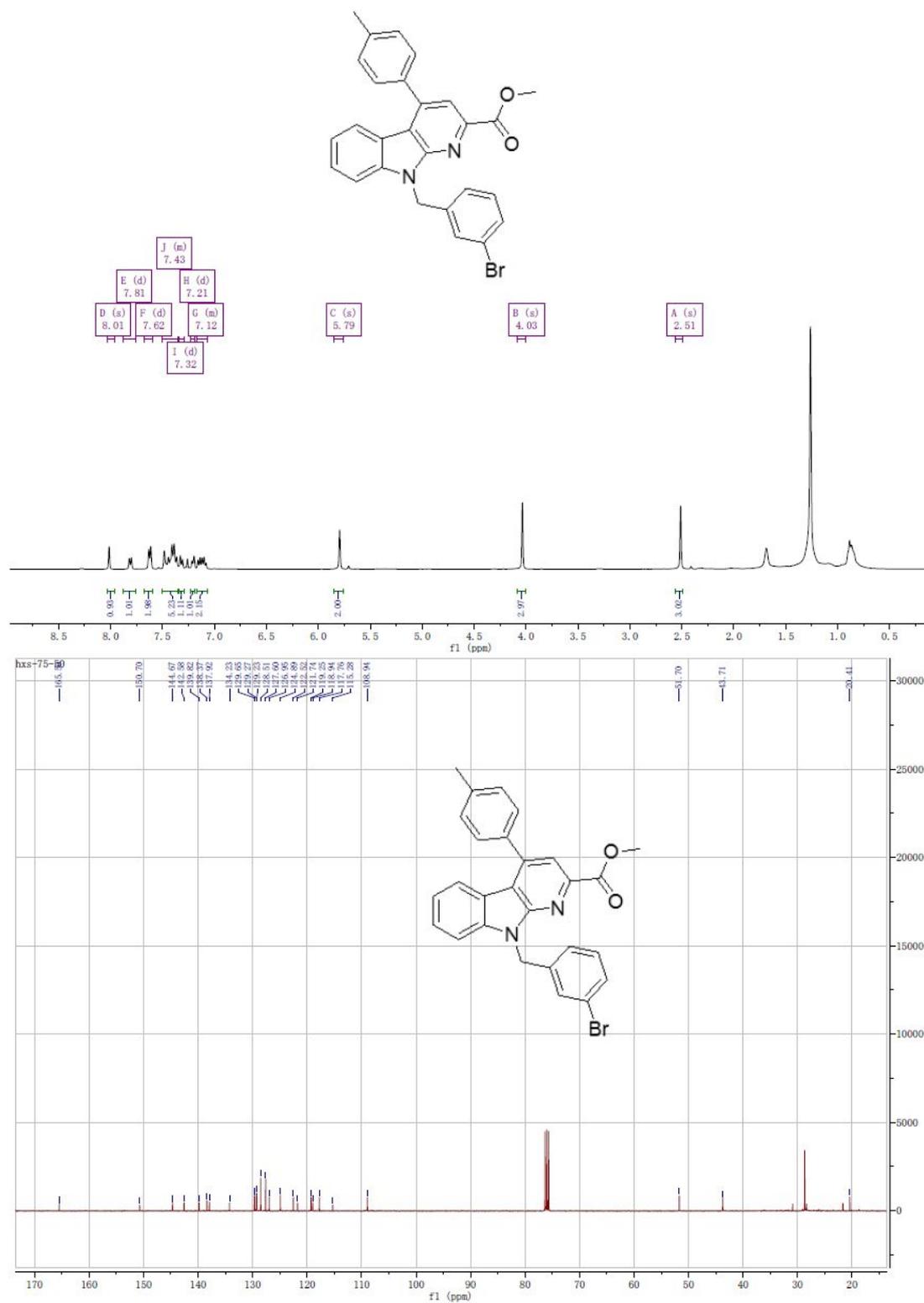
(E)-benzyl 4-(2-(furan-2-yl)vinyl)-9-methyl-9H-pyrido[2,3-b]indole-2-carboxylate (5I)

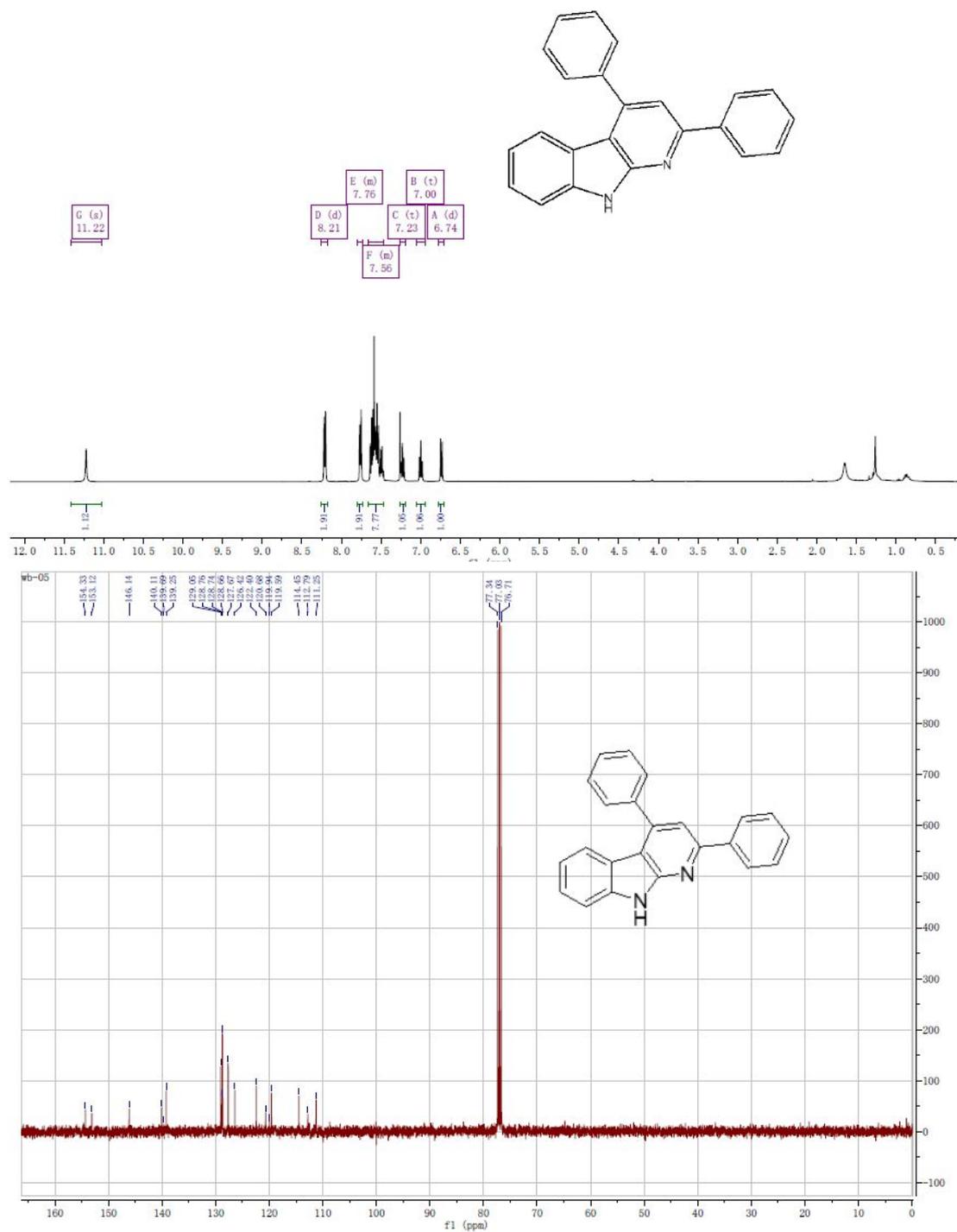


methyl 9-(4-fluorobenzyl)-4-p-tolyl-9H-pyrido[2,3-b]indole-2-carboxylate (5m)

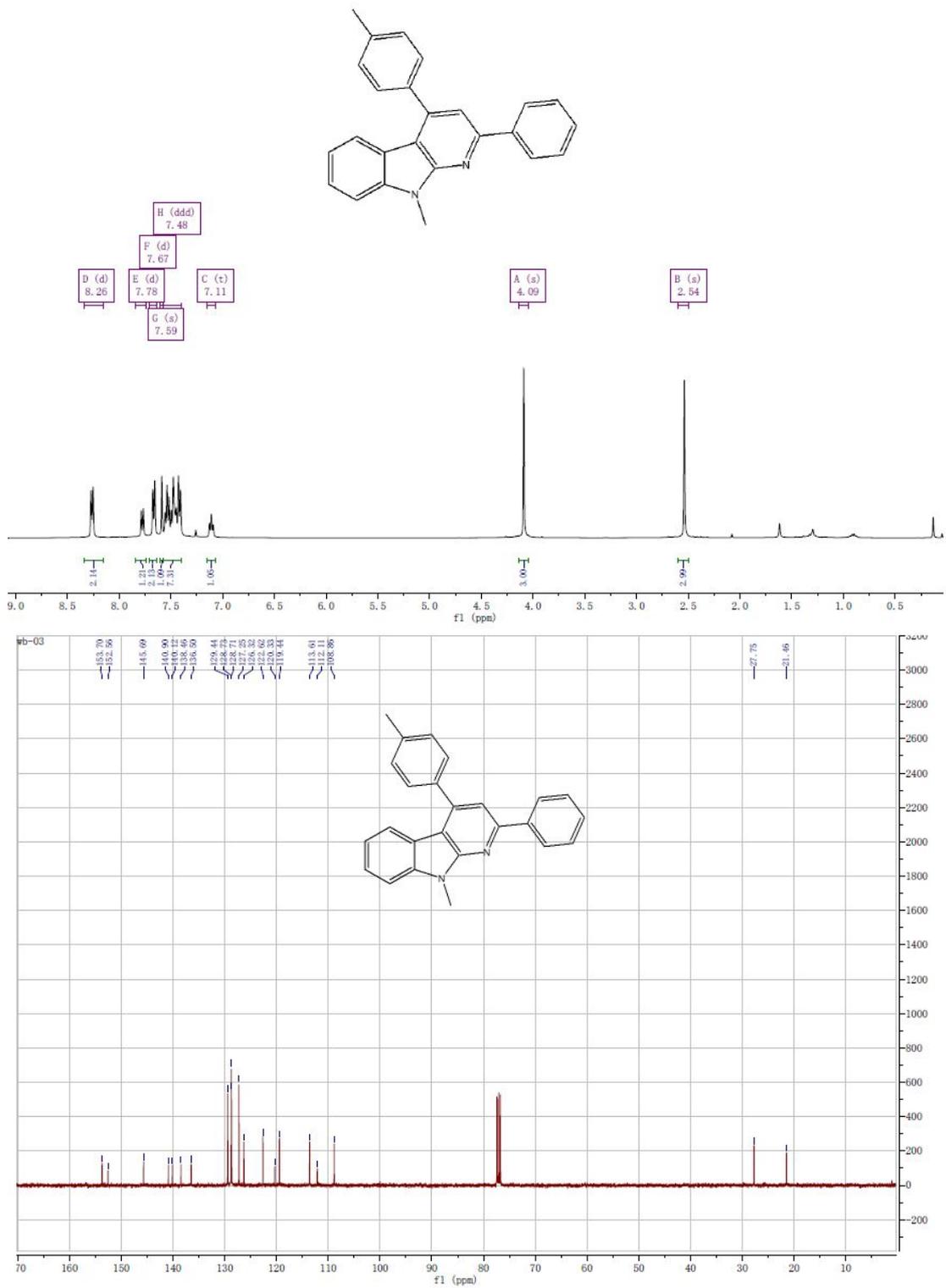


methyl 9-(3-bromobenzyl)-4-p-tolyl-9H-pyrido[2,3-b]indole-2-carboxylate (5n)

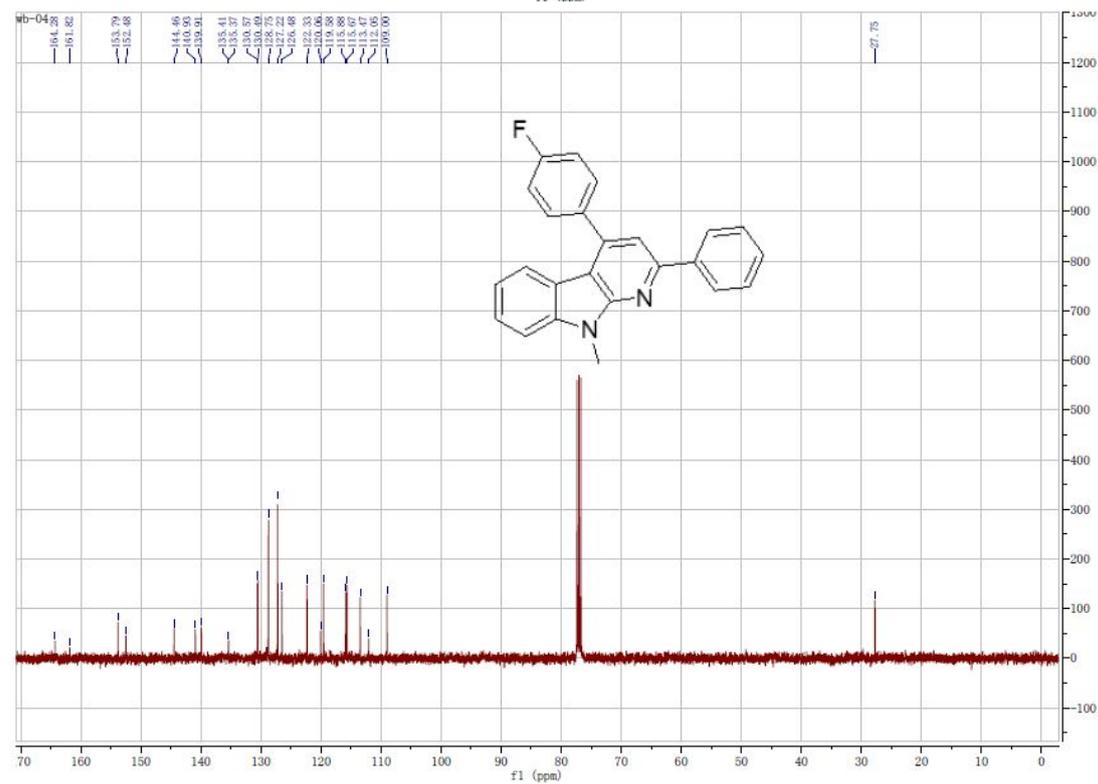
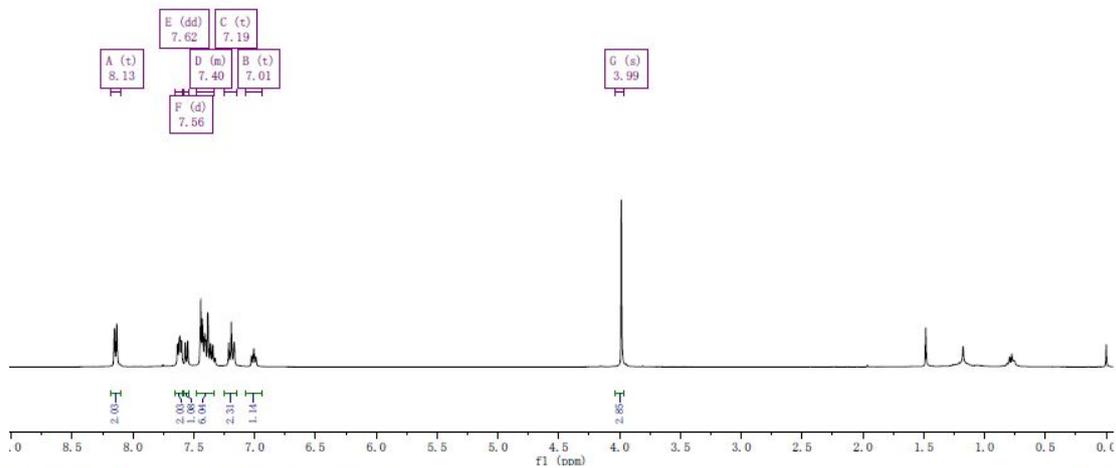
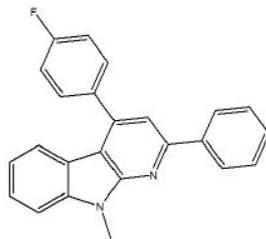




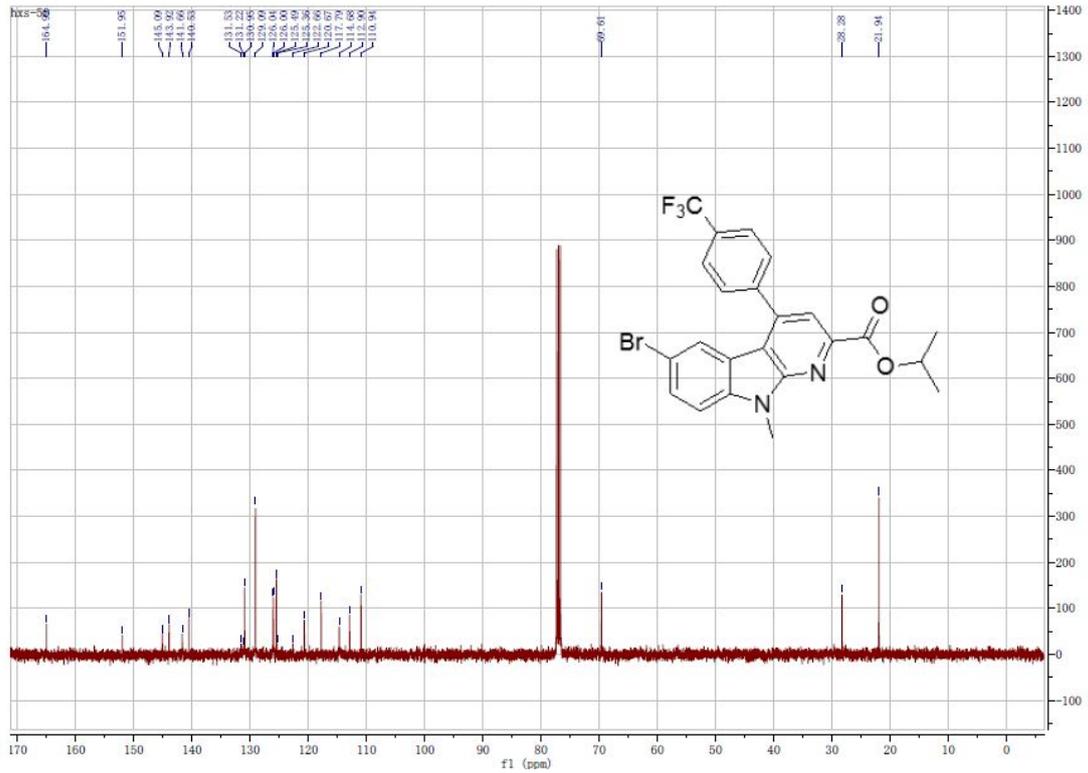
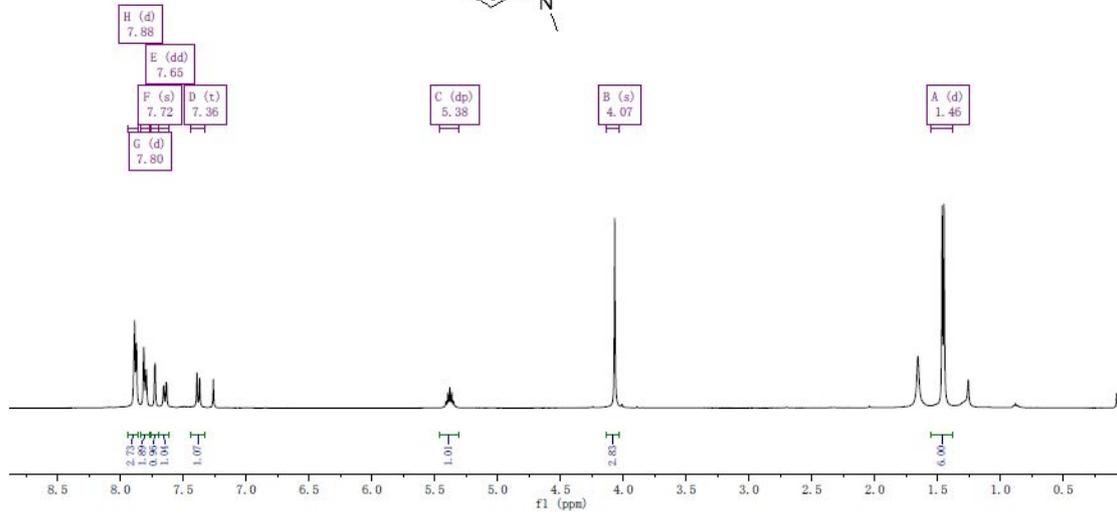
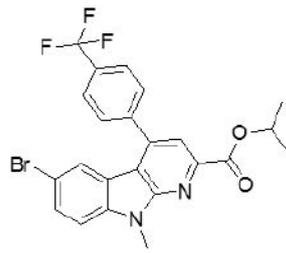
9-methyl-2,4-diphenyl-9H-pyrido[2,3-b]indole (5p)



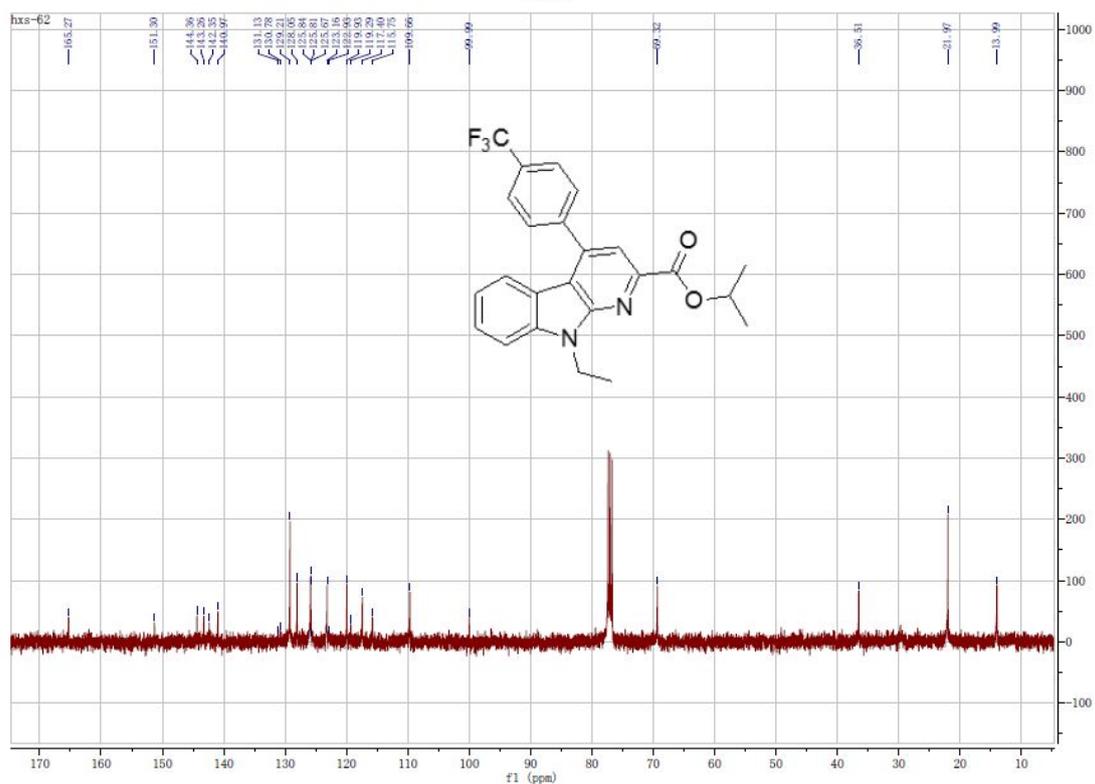
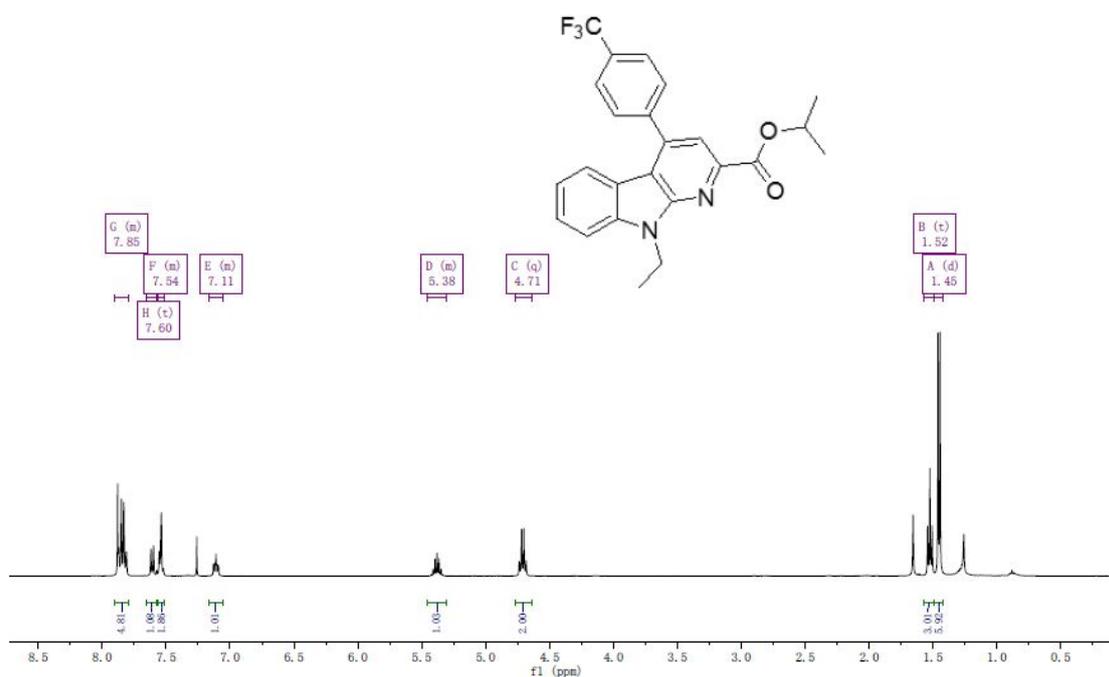
4-(4-fluorophenyl)-9-methyl-2-phenyl-9H-pyrido[2,3-b]indole (5r)



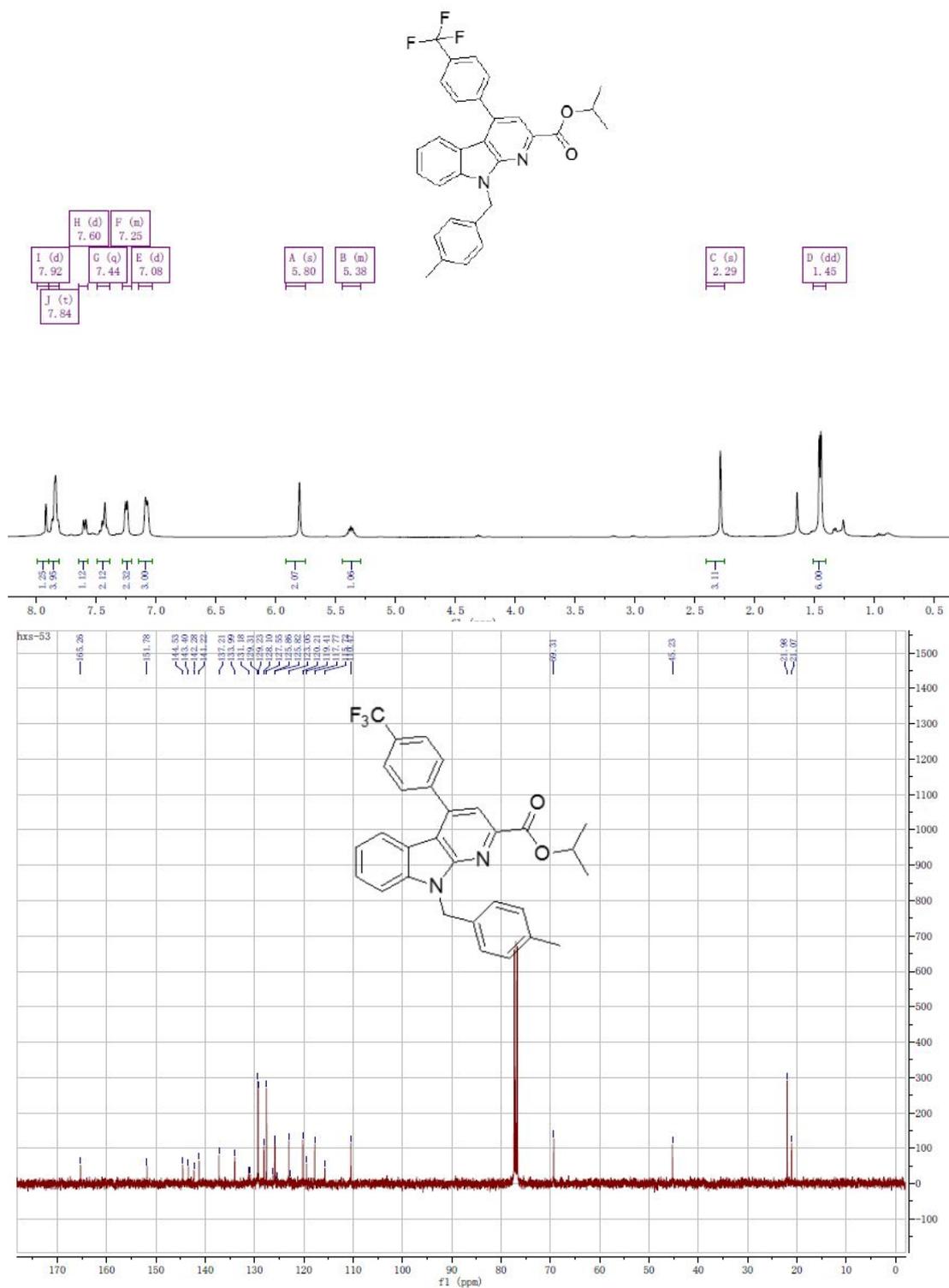
isopropyl 6-bromo-9-methyl-4-(4-(trifluoromethyl)phenyl)-9H-pyrido[2,3-b]indole-2-carboxylate (4bd)



isopropyl 9-ethyl-4-(4-(trifluoromethyl)phenyl)-9H-pyrido[2,3-b]indole-2-carboxylate (4cd)



(4ed)



isopropyl 9-(4-bromobenzyl)-4-(4-(trifluoromethyl)phenyl)-9H-pyrido[2,3-b]indole-2-carboxylate (4fd)

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