

Divergent synthesis of 1,5-benzodiazepines and benzimidazoles via a BiCl₃-catalyzed one-pot condensation–cyclization process

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Supplementary Information

Table of Contents

Crystal data and structure refinement of 3a	S2
2,2,4-trimethyl-2,3-dihydro-1H-benzo[b][1,4]diazepine	S3
2-(1-phenyl-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (5h)	S4
2-(1-(<i>p</i> -tolyl)-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (5i)	S5
Ethyl 4-(5-(1H-benzo[d]imidazol-2-yl)-2-(trifluoromethyl)-1H-imidazol-1-yl)benzoate (5j)	S6
2-(1-(<i>m</i> -tolyl)-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (5k)	S7
2-(1-([1,1'-biphenyl]-2-yl)-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (5l)	S8
7-methyl-2-(1-phenyl-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (5m)	S9
6-methyl-2-(1-phenyl-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (5n)	S10

Crystal data and structure refinement of 3a

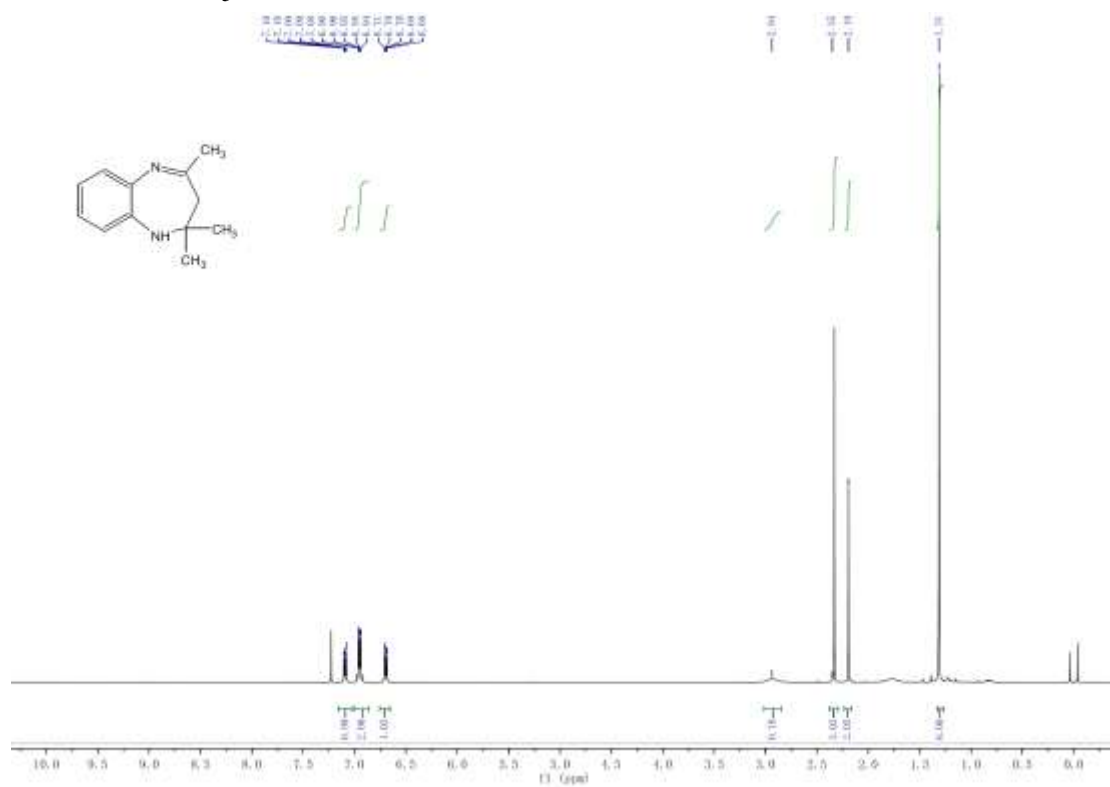
CCDC	2052113
identification code	shelx
Empirical formula	C ₁₂ H ₁₆ N ₂
Formula weight	188.27
Temperature	293(2) K
Crystal system	orthorhombic
Space group	Pna2 ₁
Unit cell dimensions	a = 12.2288(11) Å α = 90° b = 7.3218(7) Å β = 90° c = 11.9876(11) Å γ = 90°
Volume	1073.33(17) Å ³
Z	4
ρ (calc.)	1.165 g/cm ³
μ	0.535 mm ⁻¹
F(000)	408.0
Crystal size	? × ? × ? mm ³
Radiation	? (λ = 1.54059)
2θ range for data collection	14.086 to 136.27°
Index ranges	-14 ≤ h ≤ 14, -8 ≤ k ≤ 8, -14 ≤ l ≤ 13
Reflections collected	11121
Independent reflections	1953 [R _{int} = 0.0430, R _{sigma} = 0.0251]
Data/restraints/parameters	1953/1/130
Goodness-of-fit on F ²	1.254
Final R indexes [I >= 2σ (I)]	R1 = 0.0548, wR2 = 0.1177
Final R indexes [all data]	R1 = 0.0556, wR2 = 0.1184
Largest diff. peak/hole	0.34/-0.53 e Å ⁻³
Flack parameter	0.33(17)

X-ray crystal structure of 3a

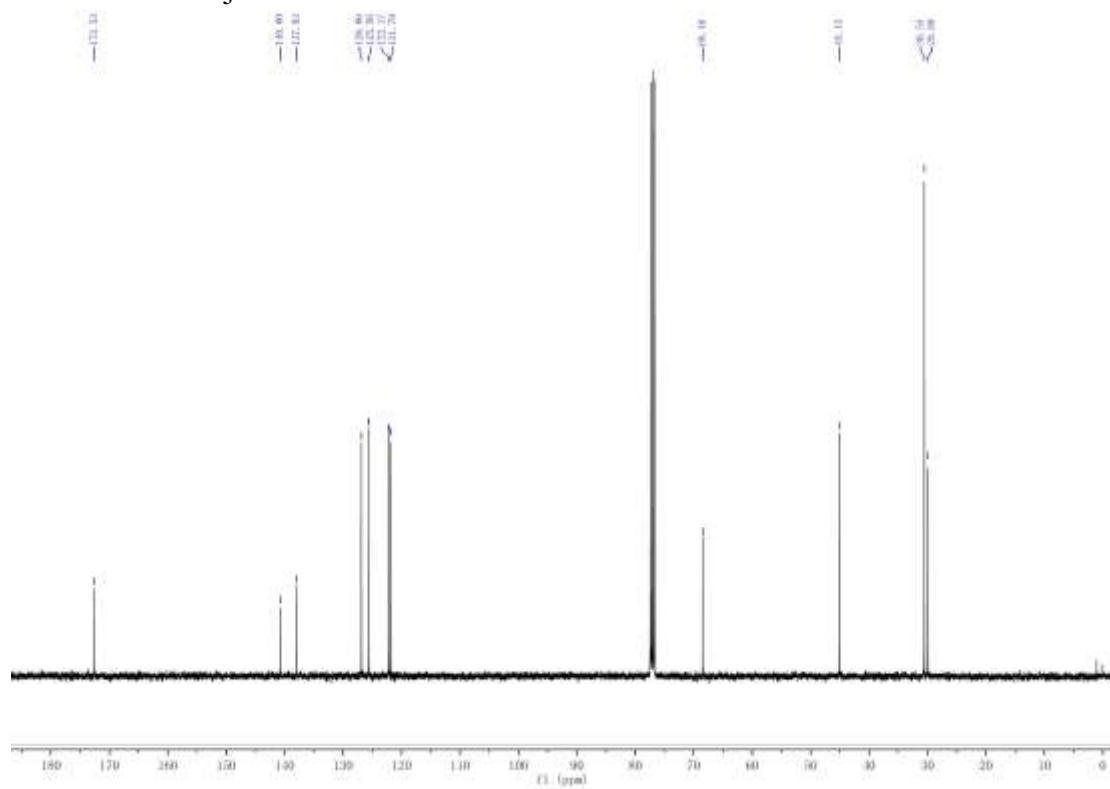


2,2,4-trimethyl-2,3-dihydro-1H-benzo[b][1,4]diazepine (3a)

^1H NMR in CDCl_3

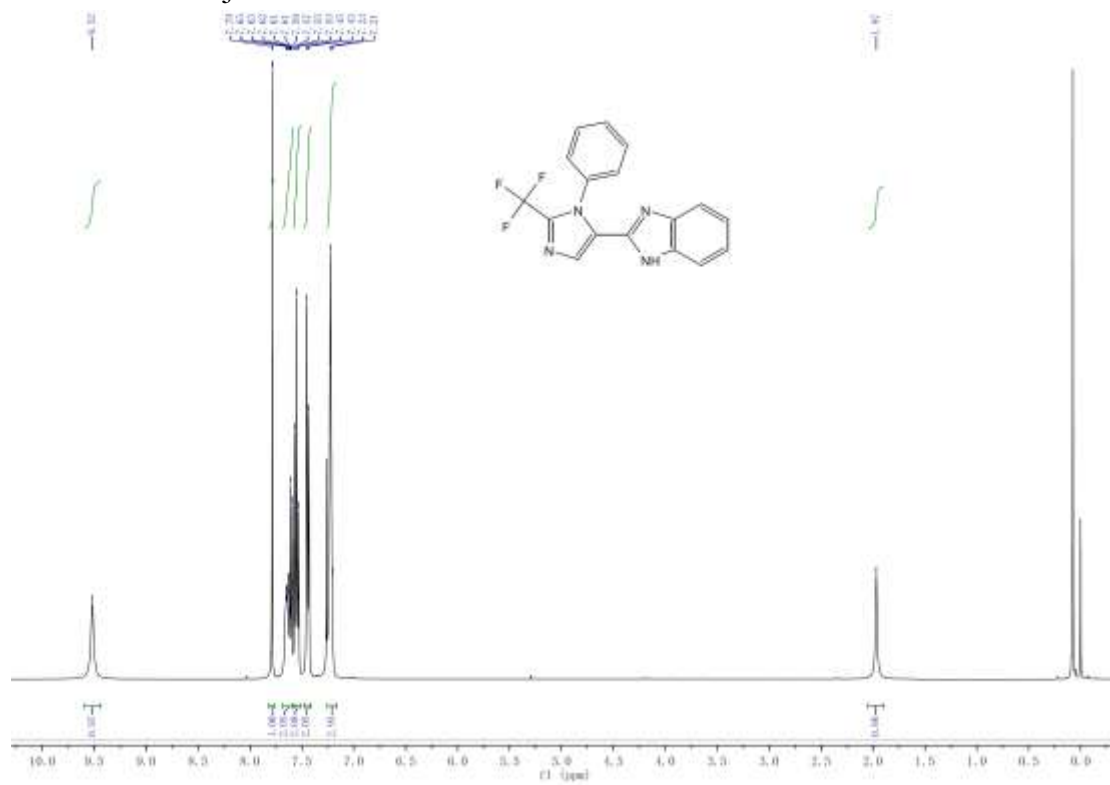


^{13}C NMR in CDCl_3

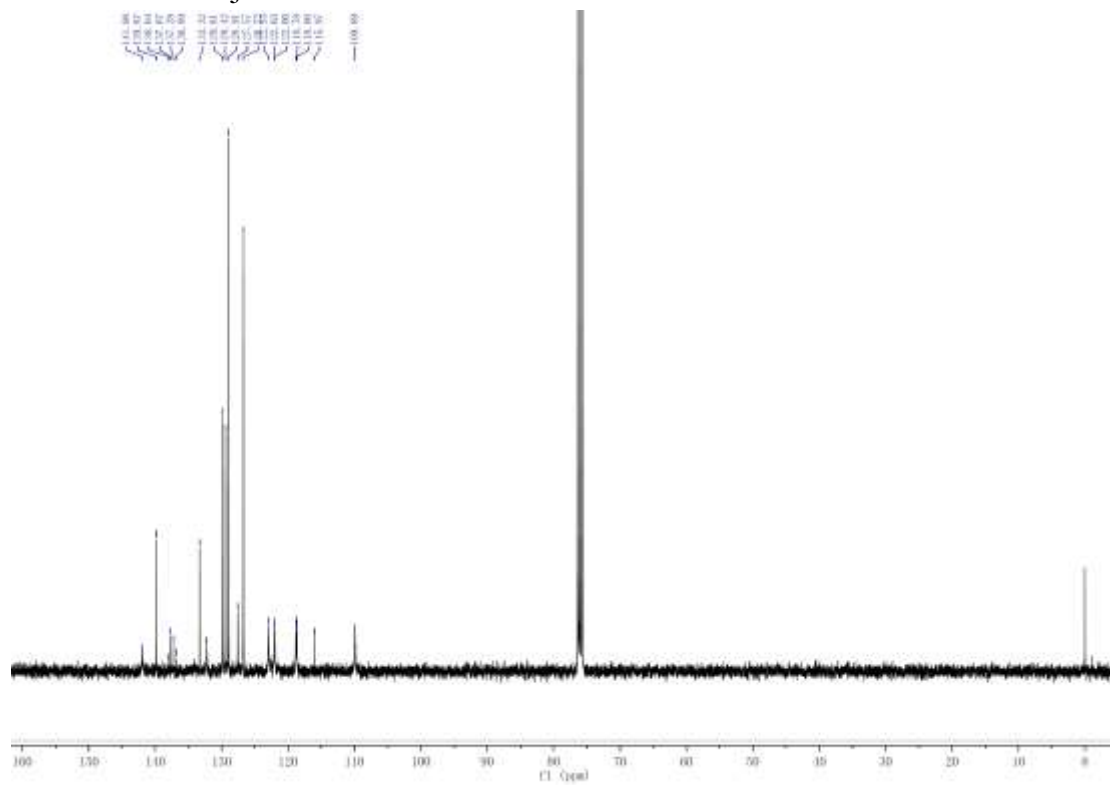


2-(1-phenyl-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (5h)

^1H NMR in CDCl_3

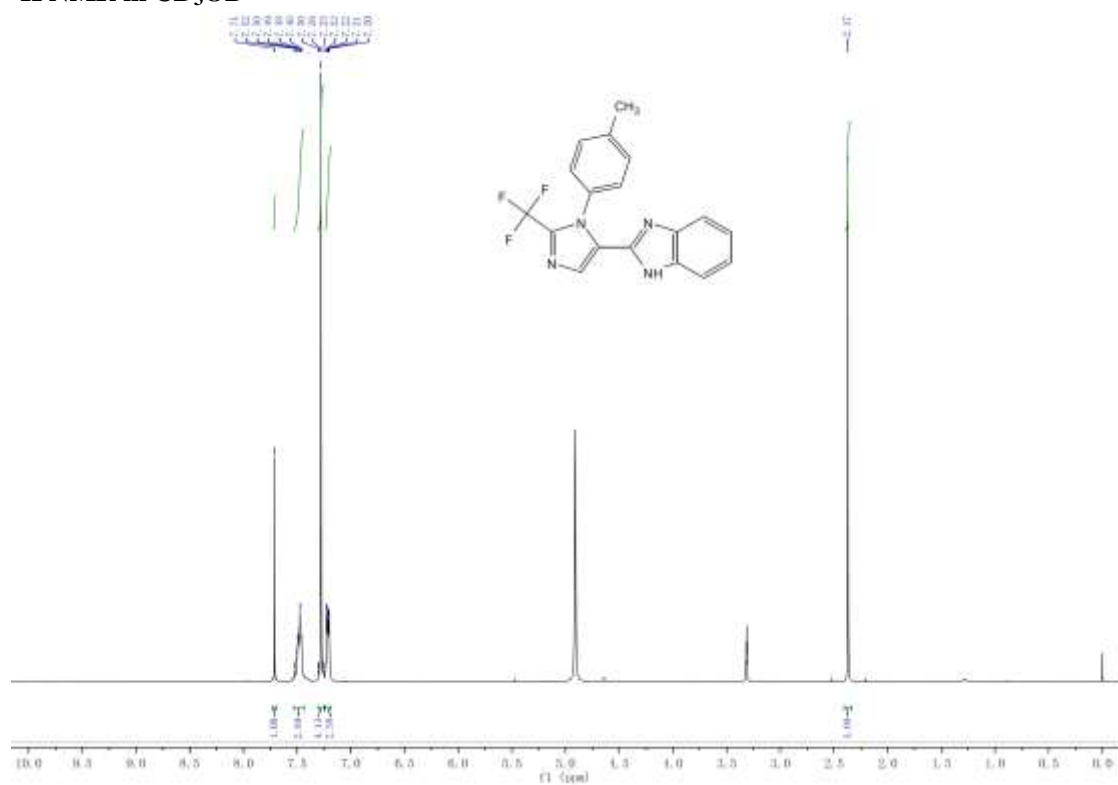


^{13}C NMR in CDCl_3

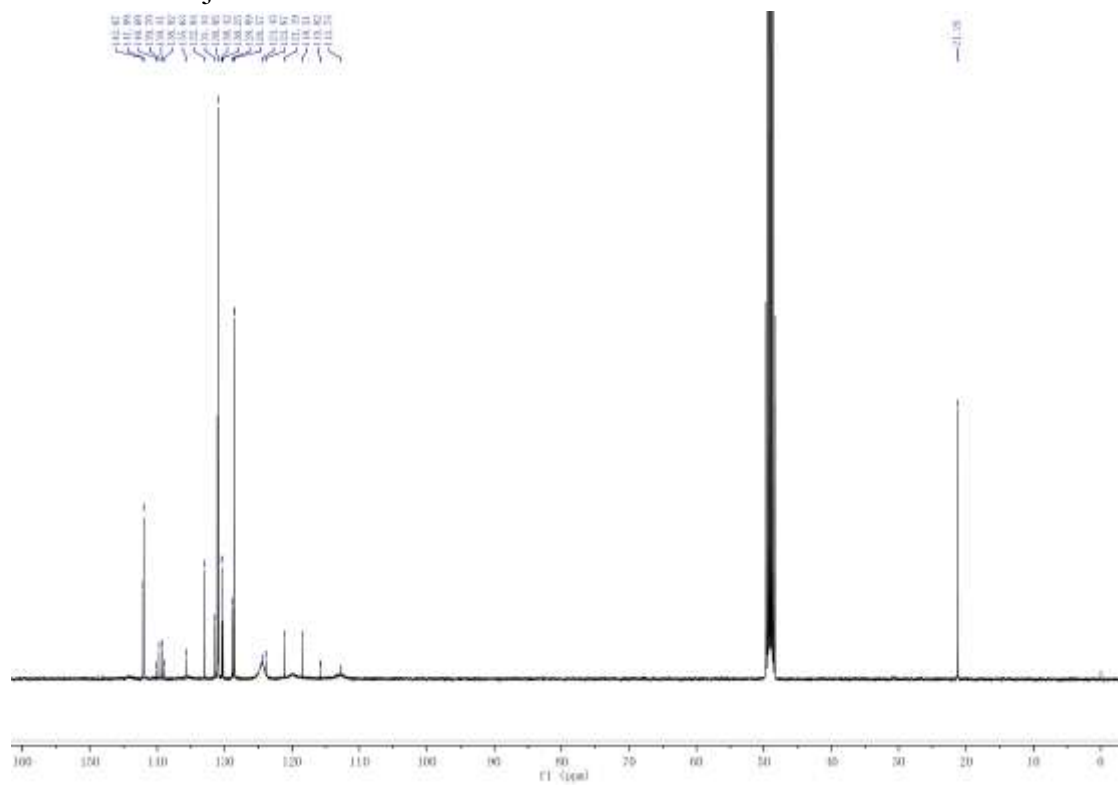


2-(1-(*p*-tolyl)-2-(trifluoromethyl)-1*H*-imidazol-5-yl)-1*H*-benzo[*d*]imidazole (5i)

^1H NMR in CD_3OD

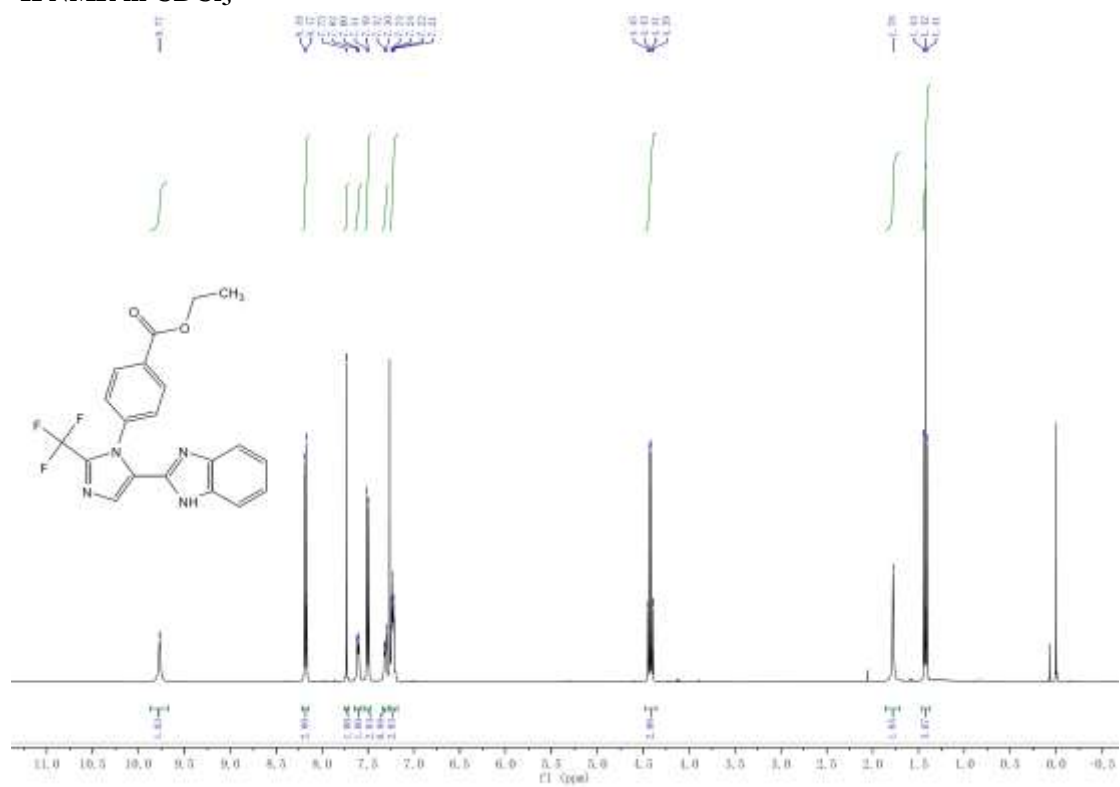


^{13}C NMR in CD_3OD

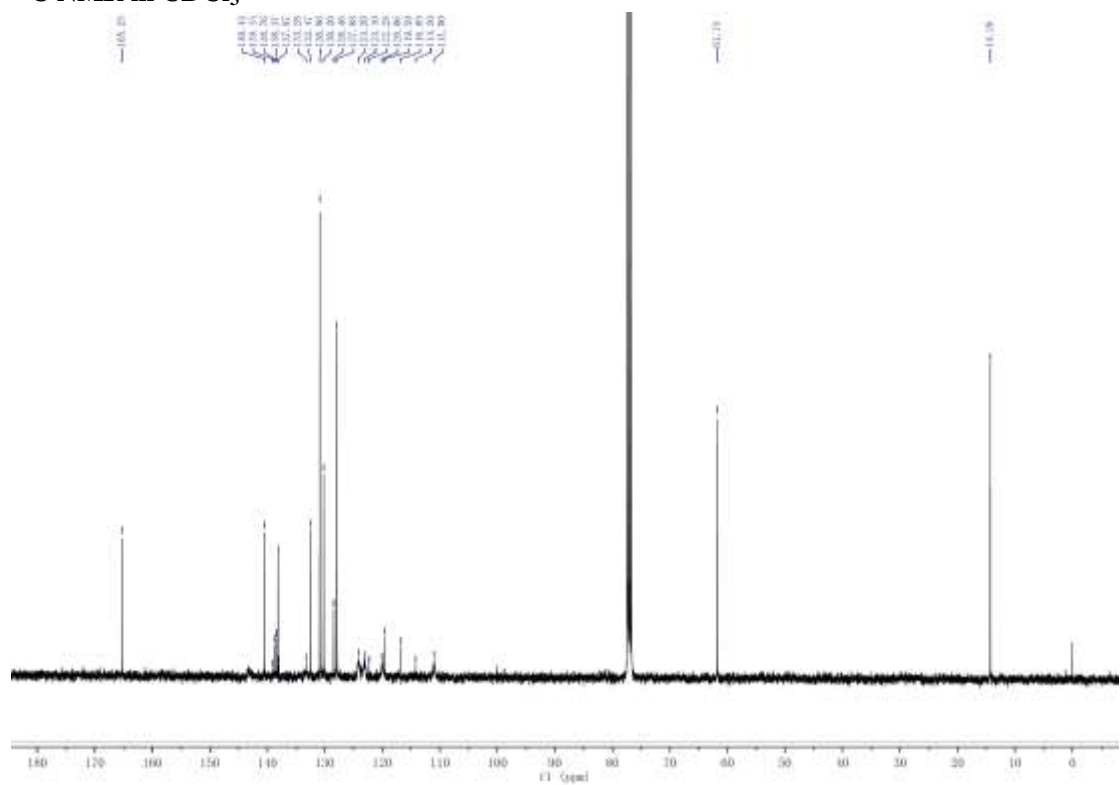


Ethyl 4-(5-(1*H*-benzo[*d*]imidazol-2-yl)-2-(trifluoromethyl)-1*H*-imidazol-1-yl)benzoate (5j)

¹H NMR in CDCl₃

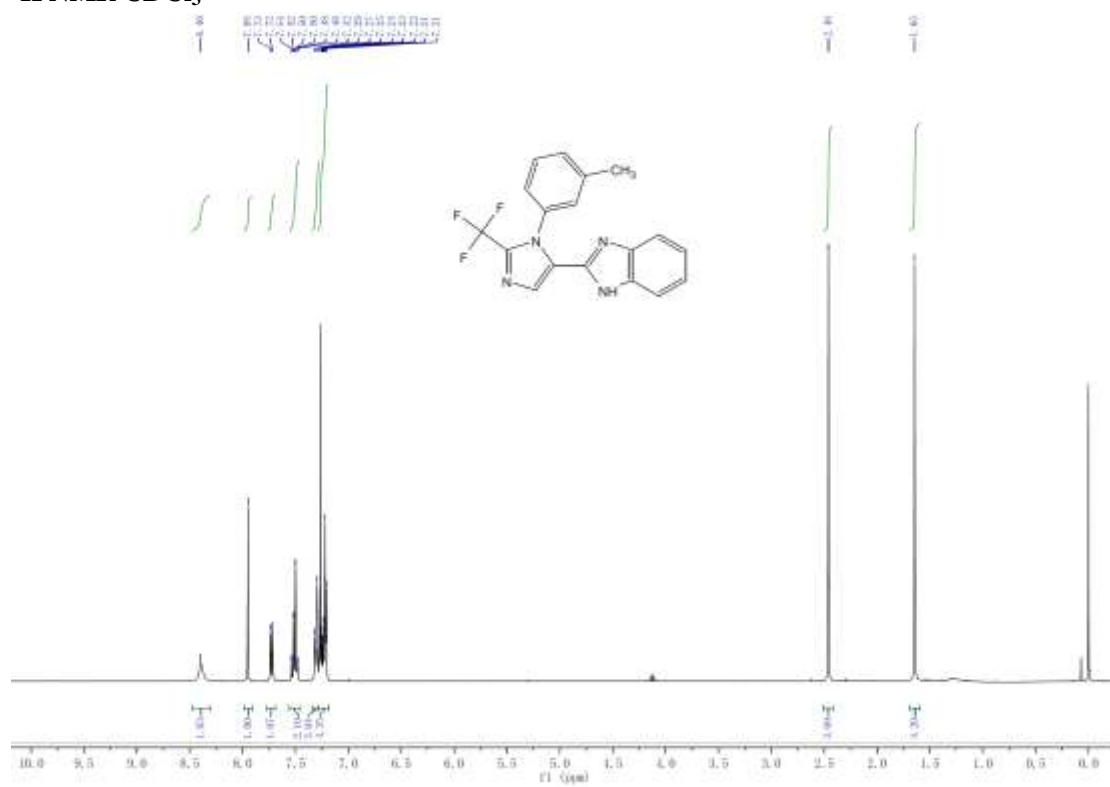


¹³C NMR in CDCl₃

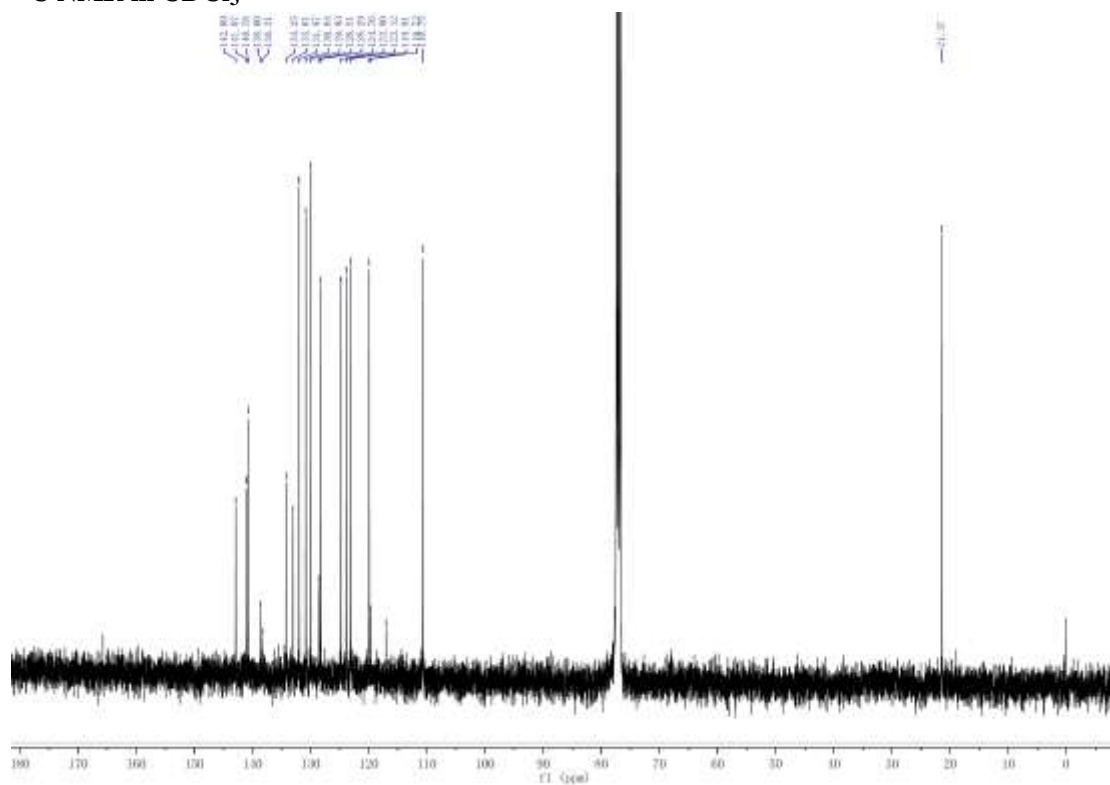


2-(1-(m-tolyl)-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (5k)

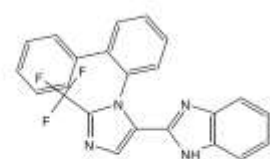
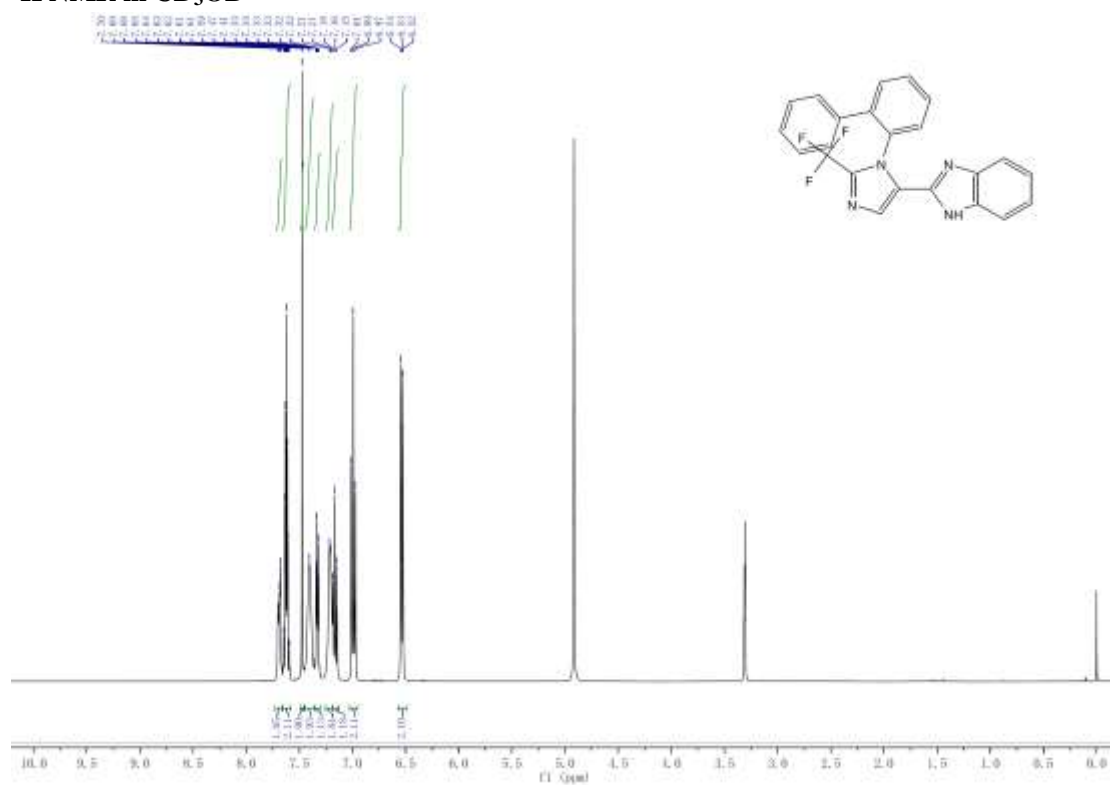
^1H NMR CDCl_3



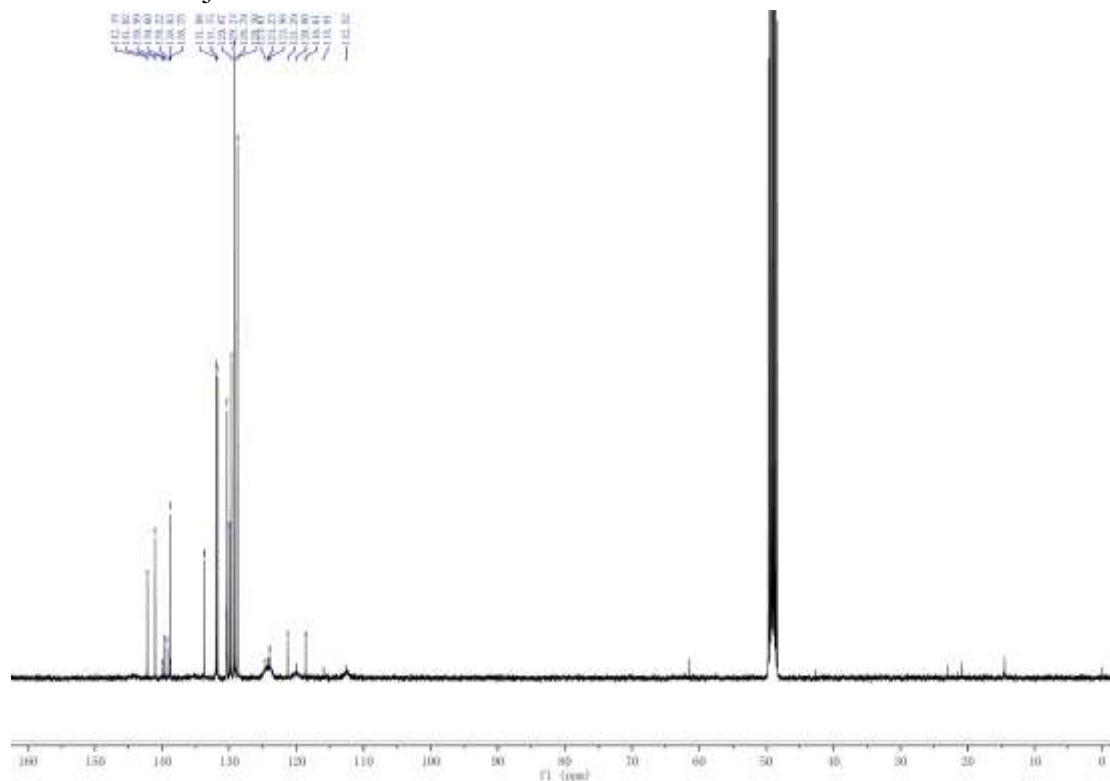
^{13}C NMR in CDCl_3



2-(1-([1,1'-biphenyl]-2-yl)-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (51)
¹H NMR in CD₃OD

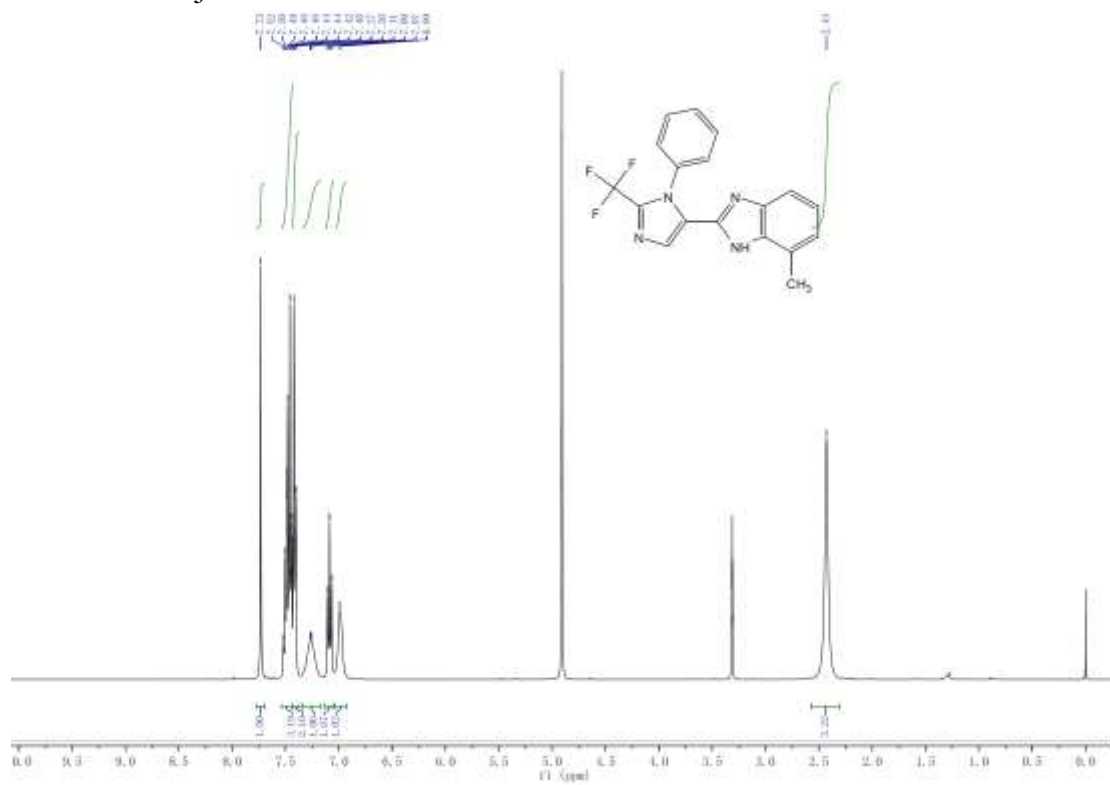


¹³C NMR in CD₃OD

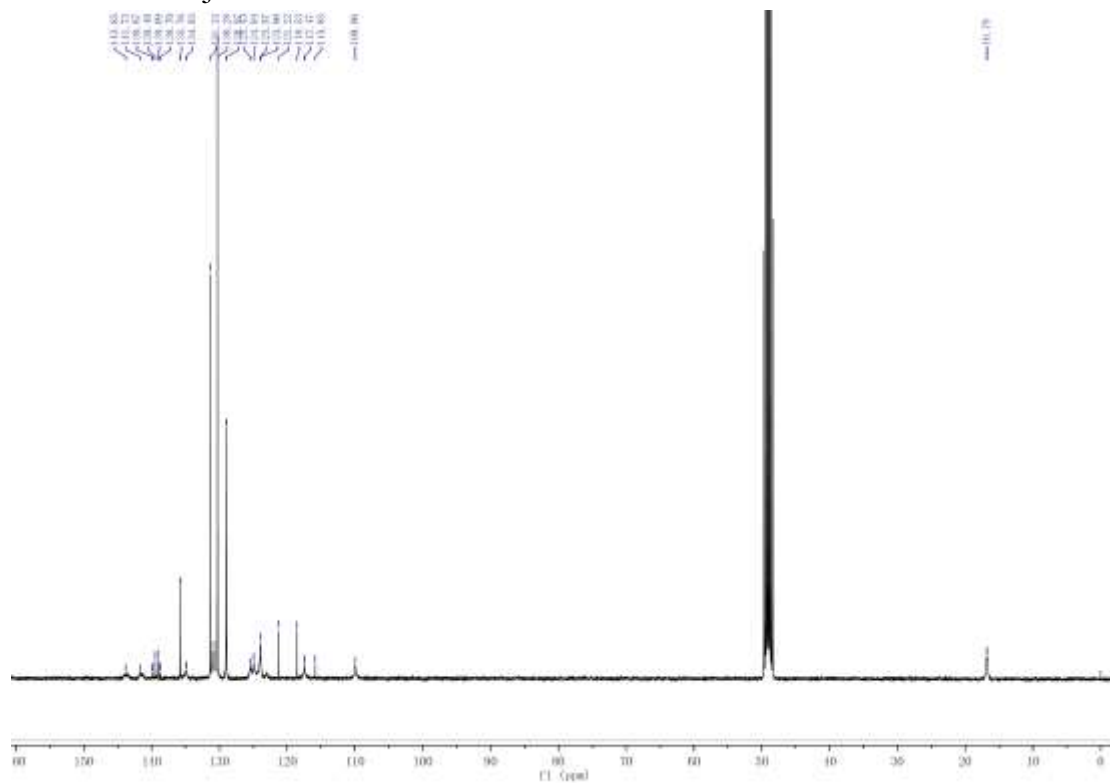


7-methyl-2-(1-phenyl-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (5m)

^1H NMR in CD_3OD

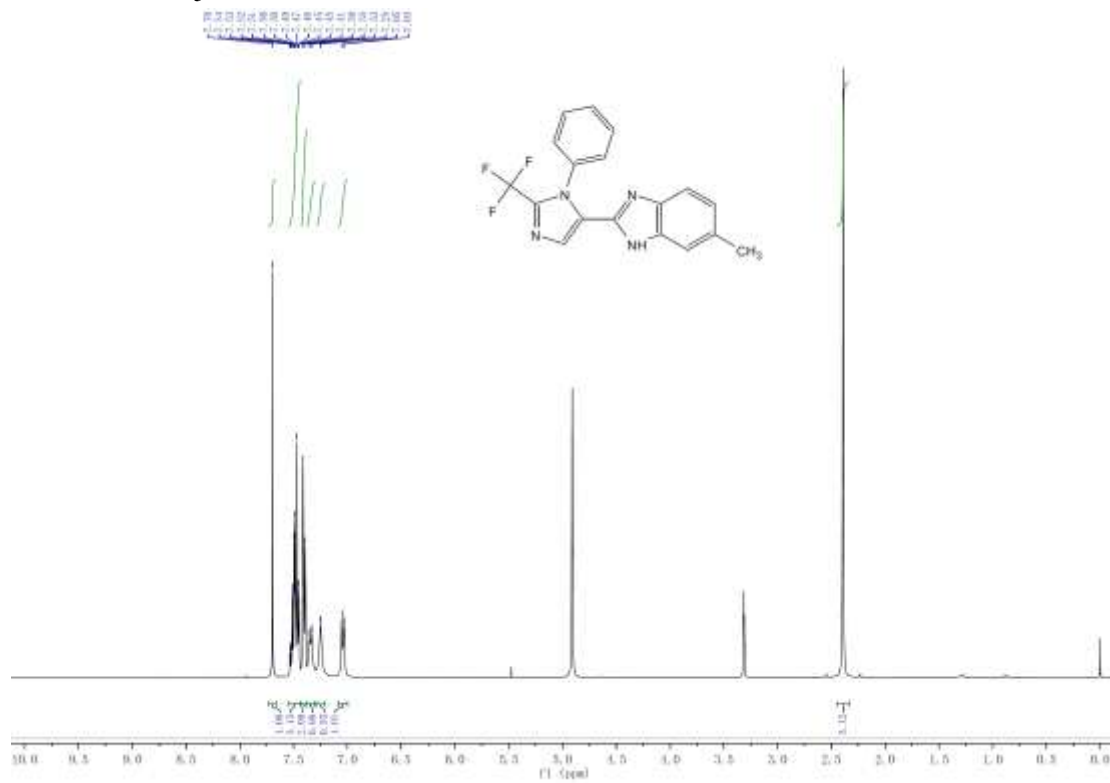


^{13}C NMR in CD_3OD



6-methyl-2-(1-phenyl-2-(trifluoromethyl)-1H-imidazol-5-yl)-1H-benzo[d]imidazole (5n)

¹H NMR in CD₃OD



¹³C NMR in CD₃OD

