

Facile regioselective on-water synthesis of 4,7-dihydropyrazolo[1,5-*a*]pyrimidines and 4,7-dihydro[1,2,4]triazolo[1,5-*a*]pyrimidines

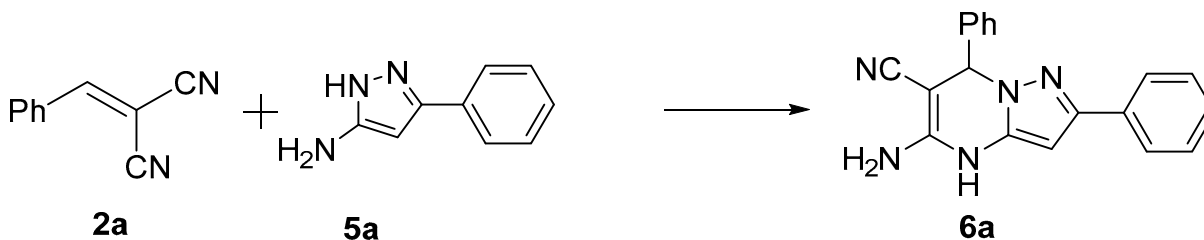
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SUPPLEMENTARY INFORMATION

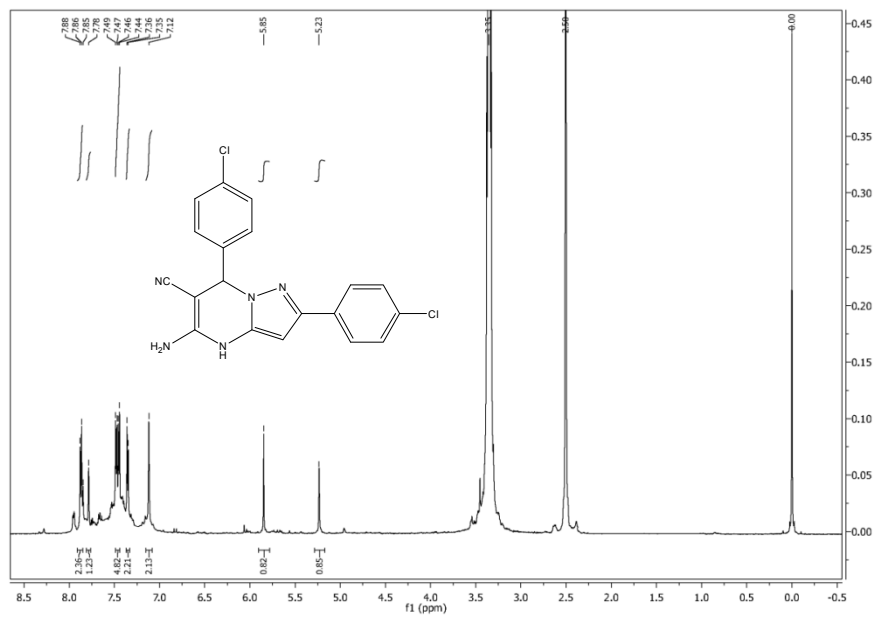
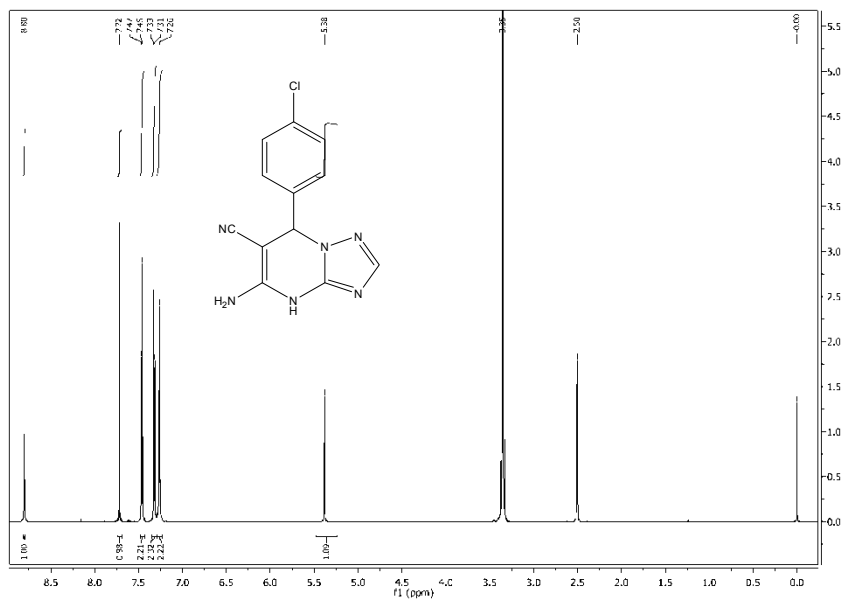
Table 1S Optimization of the reaction parameters for the synthesis of pyrazolo[1,5-*a*]pyrimidine^a

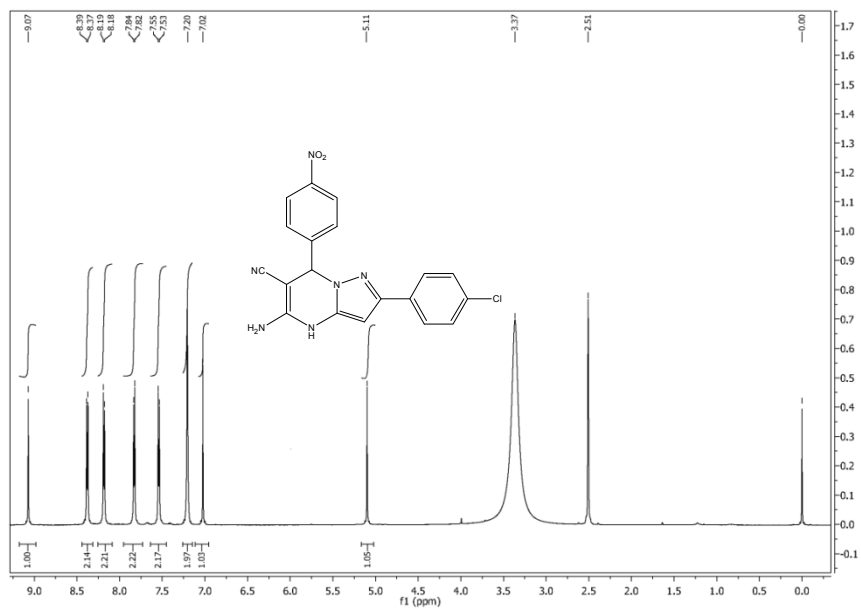


Entry	Solvent	Catalyst (mol%)	Temp. (°C)	Time	Yield* (%)
1.	MeOH	Cs ₂ CO ₃ (10)	rt (stirring)	8h	65 ^{b,c}
2.	MeOH	Cs ₂ CO ₃ (10)	reflux ^d	6h	71 ^{b,c}
3.	MeOH:Water (4:1)	Cs ₂ CO ₃ (10)	rt (stirring)	8h	^{c,e} Poor
4.	MeOH:Water (4:1)	Cs ₂ CO ₃ (10)	reflux ^d	8h	^{c,e} Poor
5.	MeOH	DBU (5)	reflux ^d	1h	70 ^b
6.	MeOH	DBU (10)	reflux ^d	1h	71 ^b
7.	MeOH:Water (4:1)	DBU (5)	reflux ^d	35 min	79 ^b
8.	MeOH:Water (4:1)	DBU (10)	reflux ^d	31min	84 ^b
9.	Water	DBU (5)	reflux ^d	30min	79 ^b
10.	Water	DBU (10)	reflux ^d	24min	82 ^b

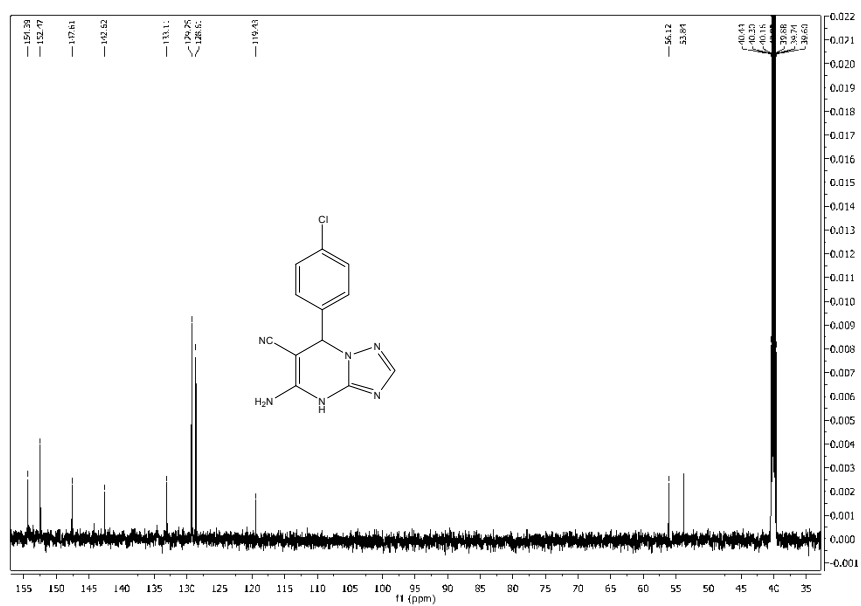
^aReaction conditions: 2-benzylidenemalononitrile **2a** (84 mg, 1 mmol), 3-phenyl-1*H*-pyrazol-5-amine **5a** (159 mg, 1 mmol), ^bIsolated yield, ^cFully conjugated pyrazolo[1,5-*a*]pyrimidine was obtained. ^dConventional heating, ^eYield is given for the crude product*Analyzed by ¹H NMR.

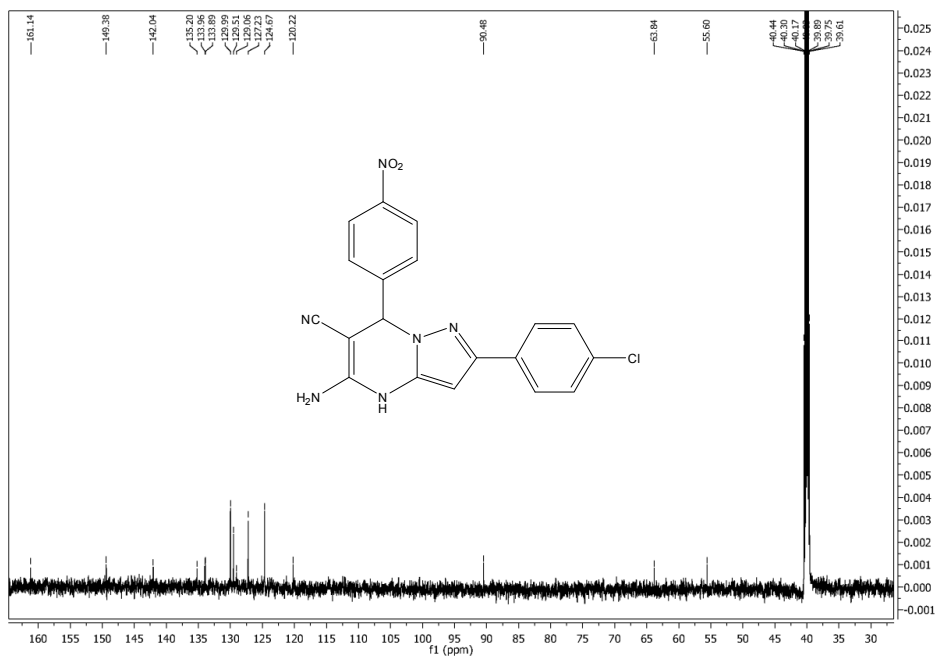
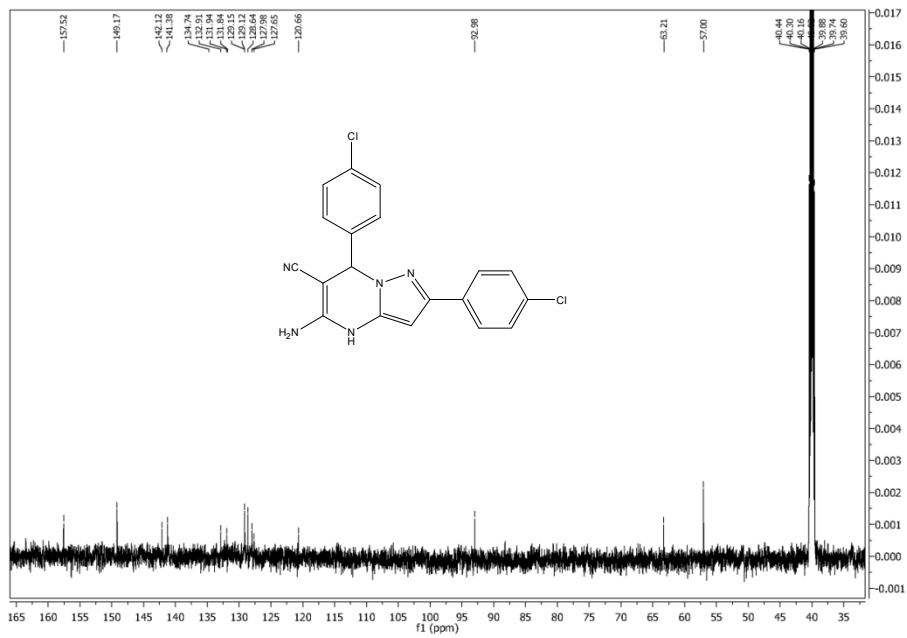
¹H NMR Spectra of synthesized compounds



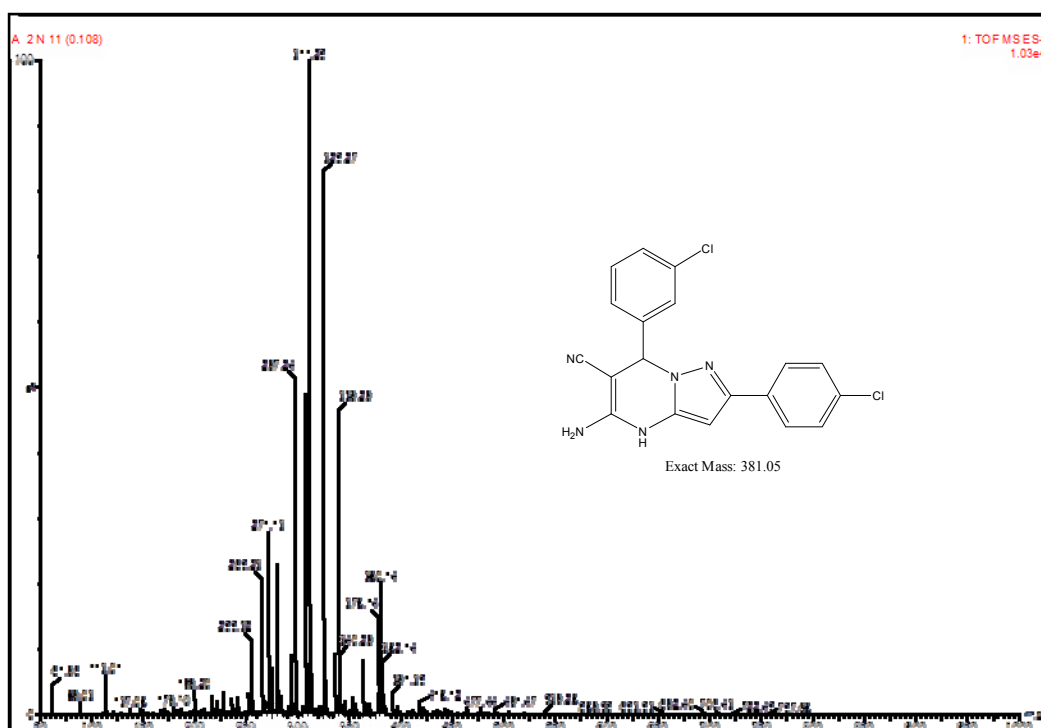
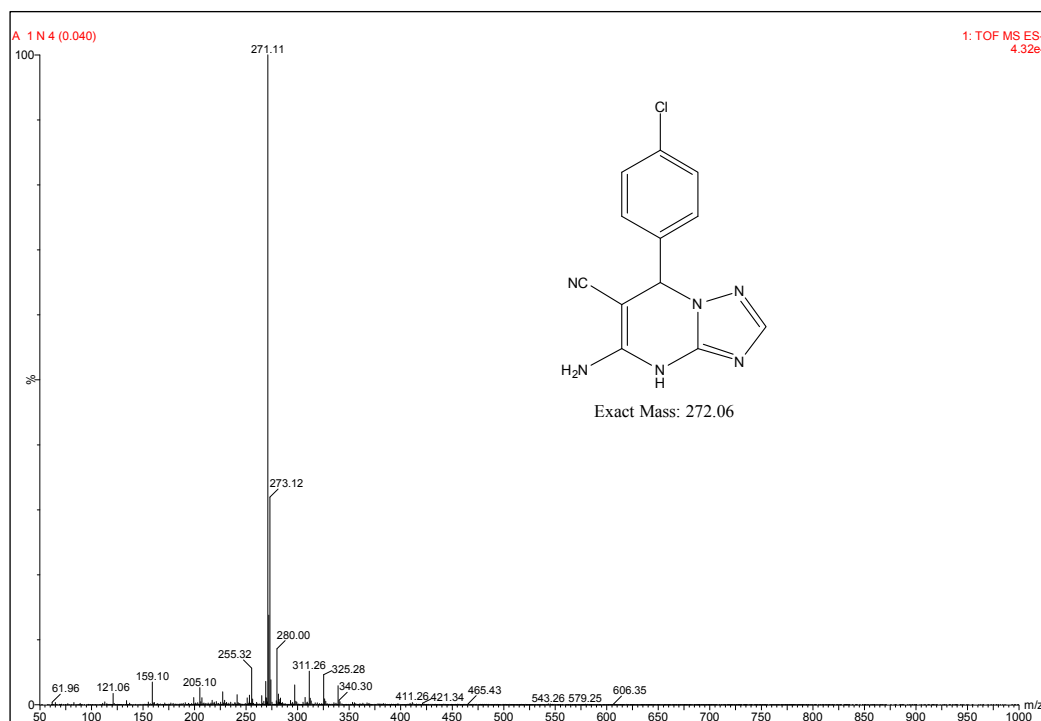


¹³C NMR Spectra of synthesized compounds





Mass Spectra of synthesized compounds



FTIR Spectra of synthesized compounds

