

Supporting Information
for
IBD-mediated oxidative cyclization of
pyrimidinylhydrazones and concurrent Dimroth
rearrangement: Synthesis of
[1,2,4]triazolo[1,5-c]pyrimidine derivatives

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200433 Shanghai, P. R. China

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*Corresponding author

NMR spectral data for unknown compounds

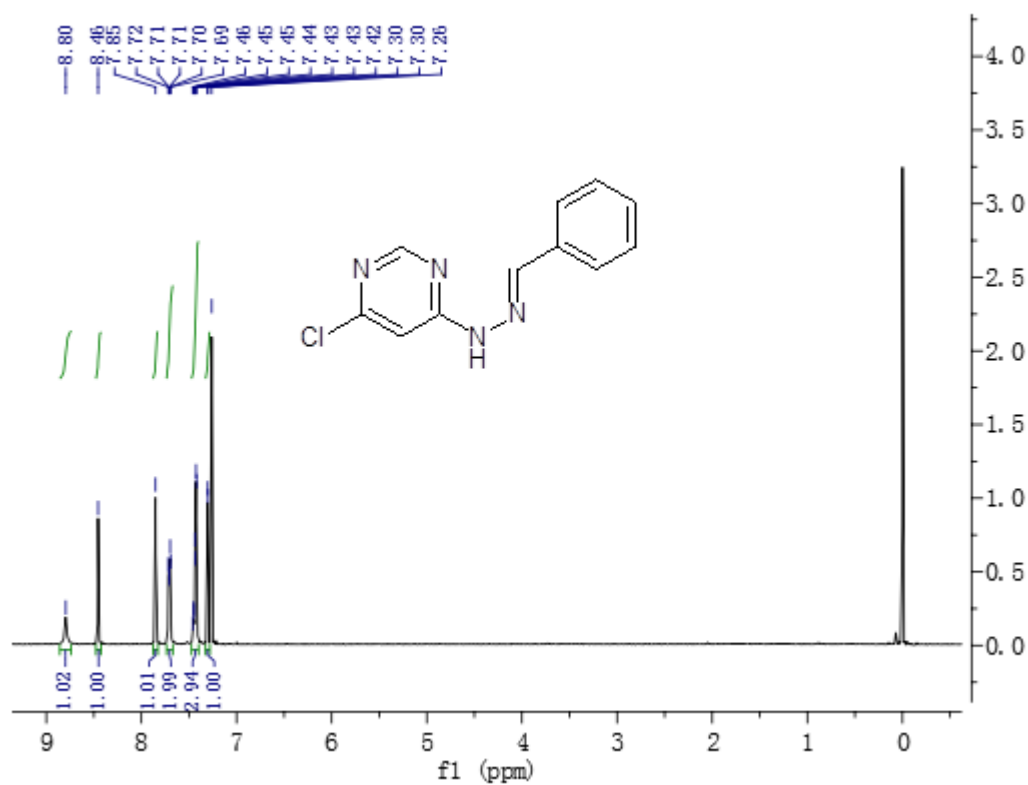
Spectra of (6-chloro-4-pyrimidinyl)hydrazones **4**..... S2

Spectra of 7-chloro-5-methyl-3-phenyl[1,2,4]triazolo[4,3-c]pyrimidine (**5f**).....S15

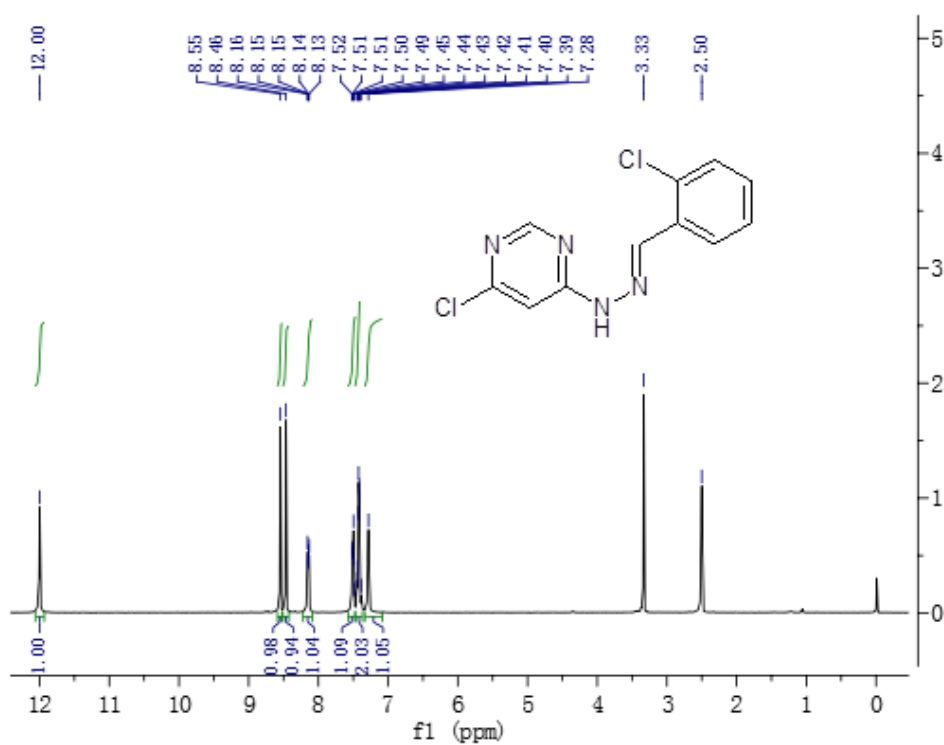
Spectra of 7-chloro-[1,2,4]triazolo[1,5-c]pyrimidines **6**..... S16

Spectra of (6-chloro-4-pyrimidinyl)hydrazones 4

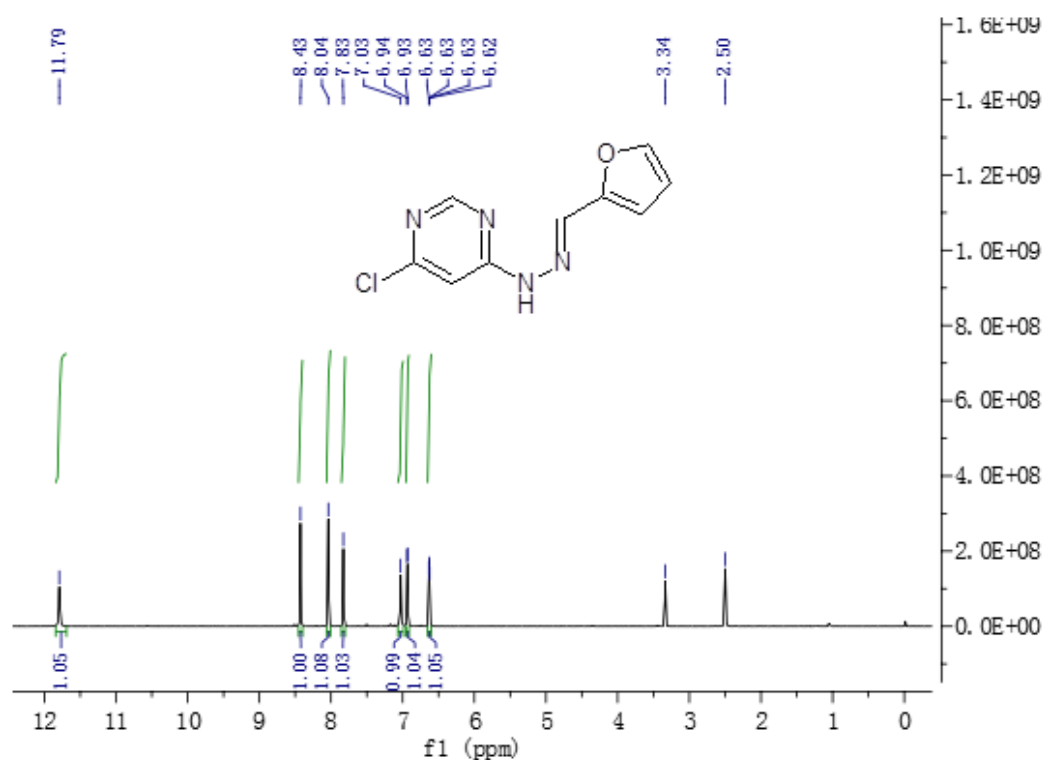
Benzaldehyde (6-chloro-4-pyrimidinyl)hydrazone (4a)



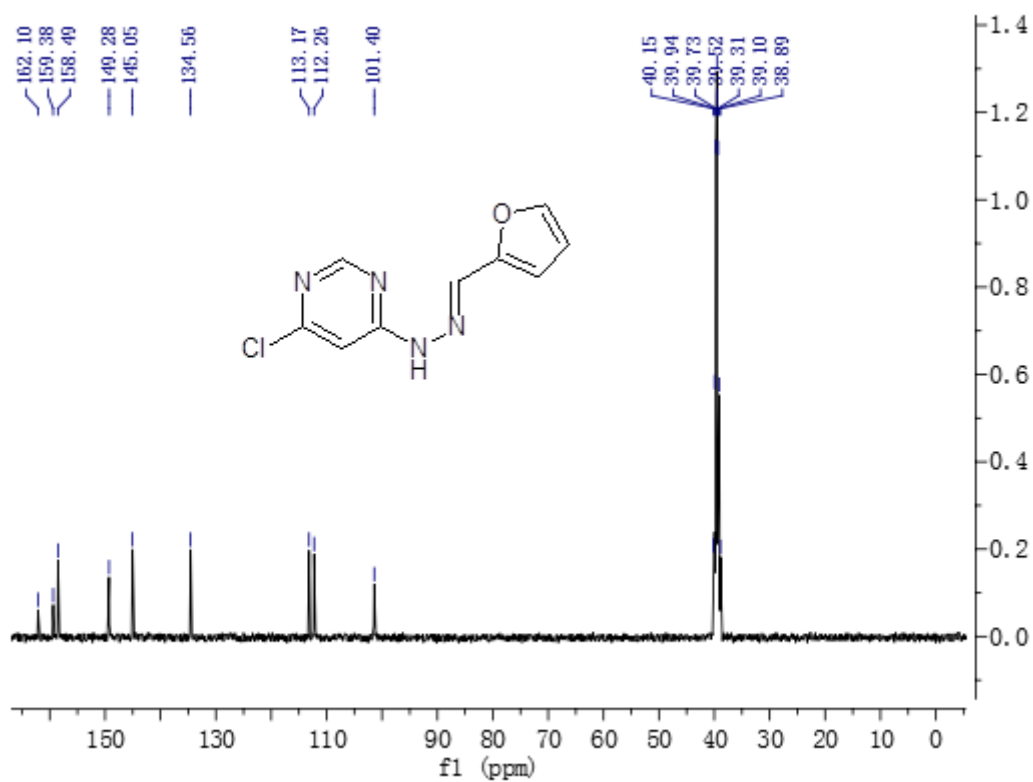
2-Chlorobenzaldehyde (6-chloro-4-pyrimidinyl)hydrazone (4b)



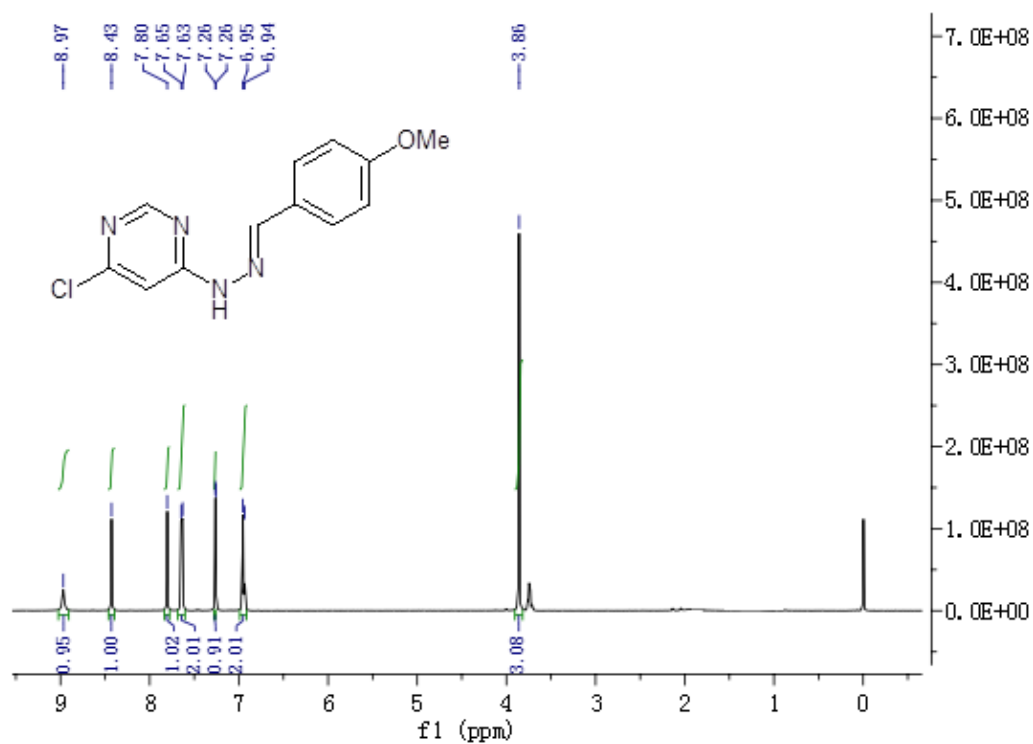
Furfural (6-chloro-4-pyrimidinyl)hydrazone (4c)



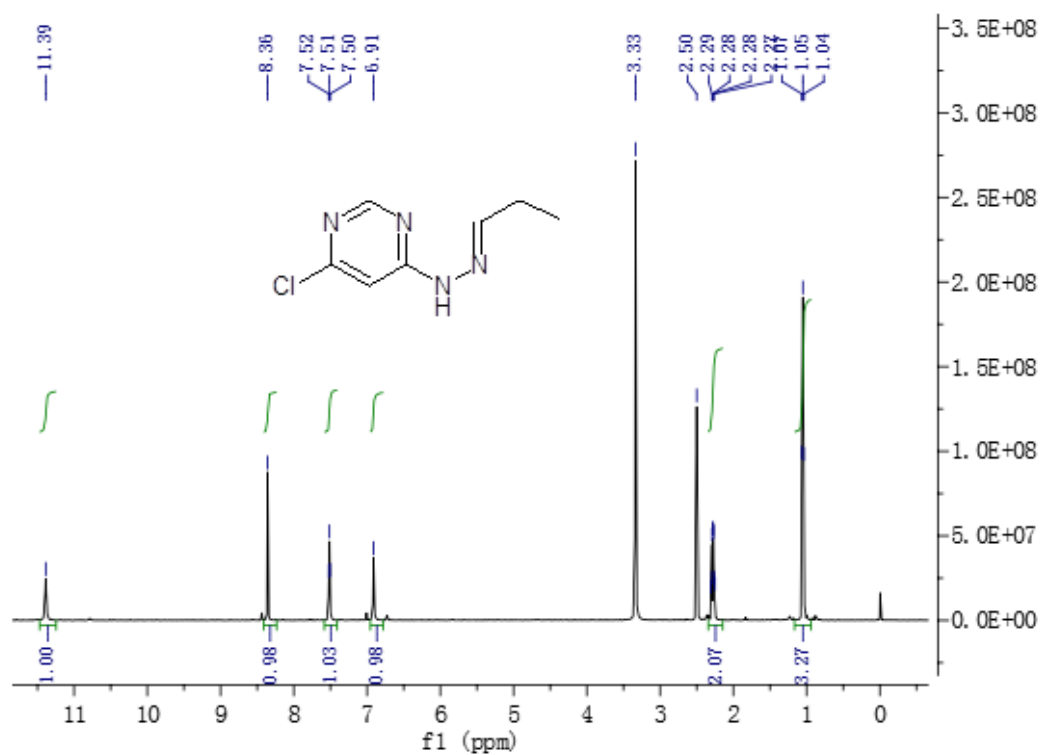
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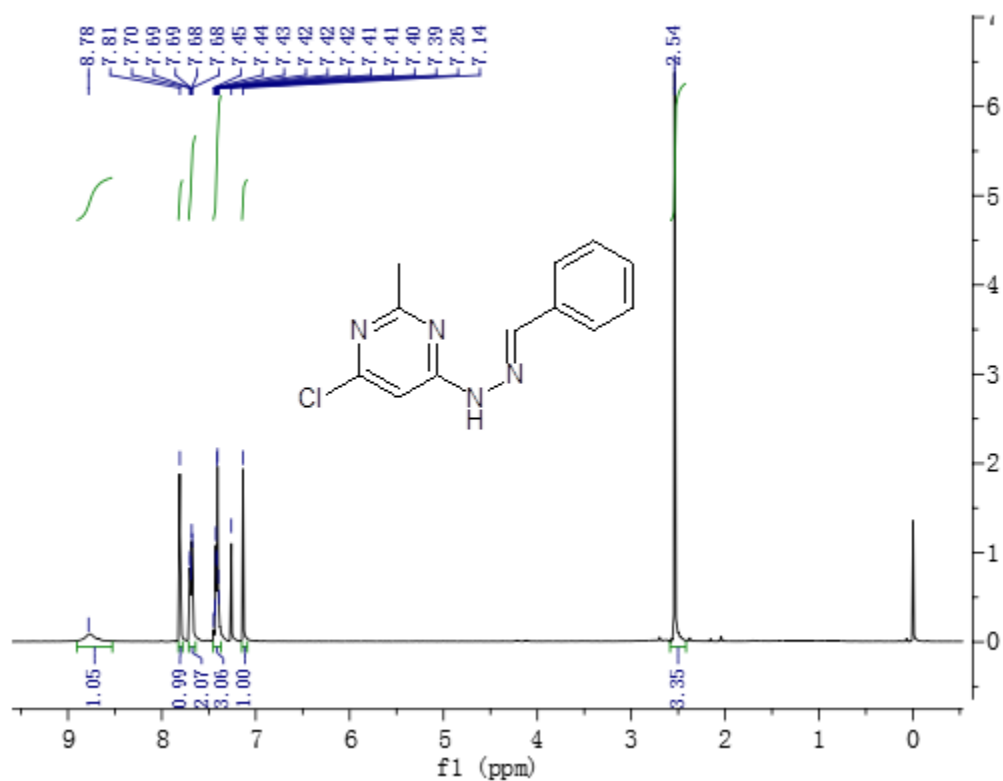
4-Methoxybenzaldehyde (6-chloro-4-pyrimidinyl)hydrazone (4d)



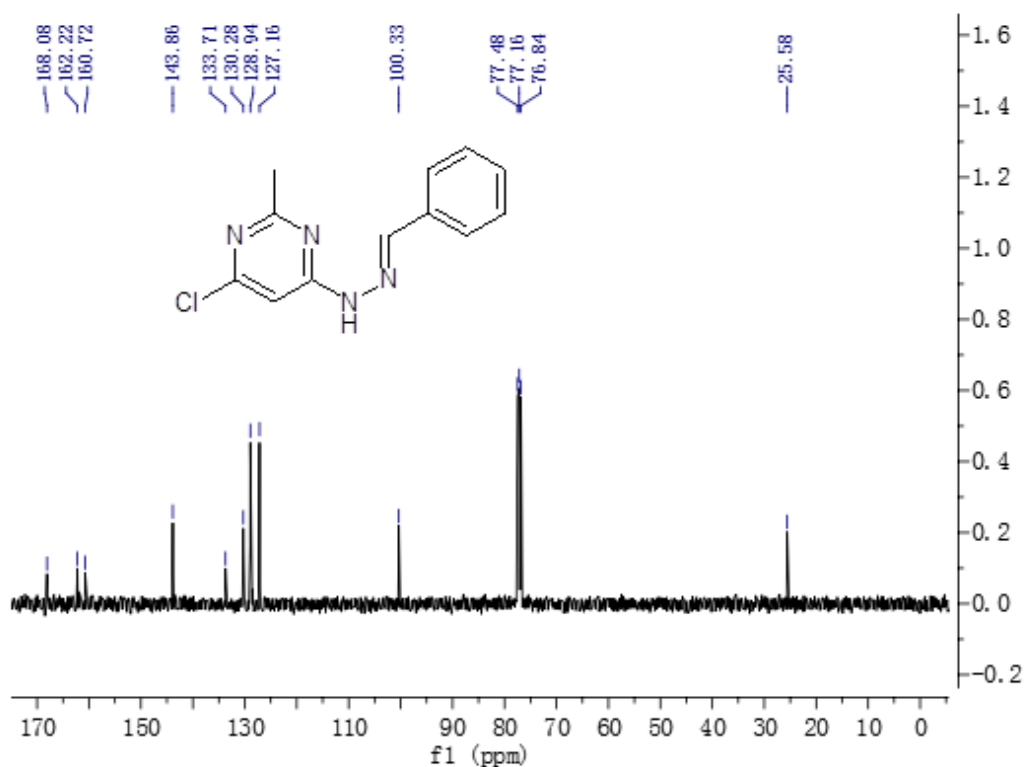
Propanaldehyde (6-chloro-4-pyrimidinyl)hydrazone (4e)



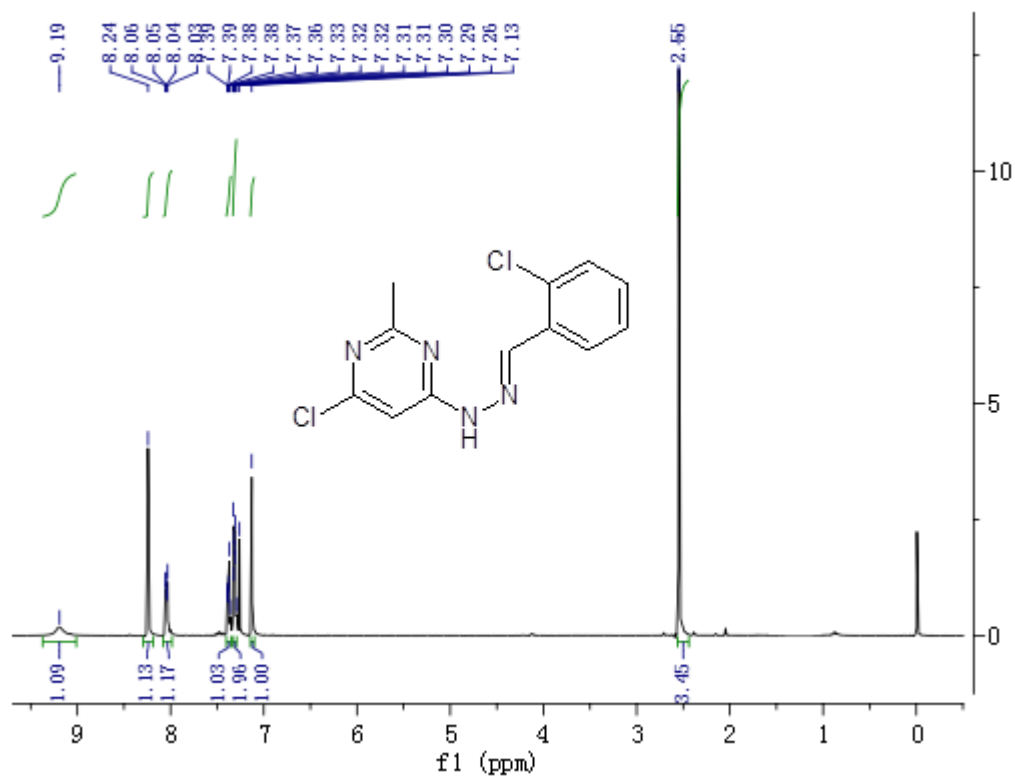
Benzaldehyde (6-chloro-2-methyl-4-pyrimidinyl)hydrazone (4f)



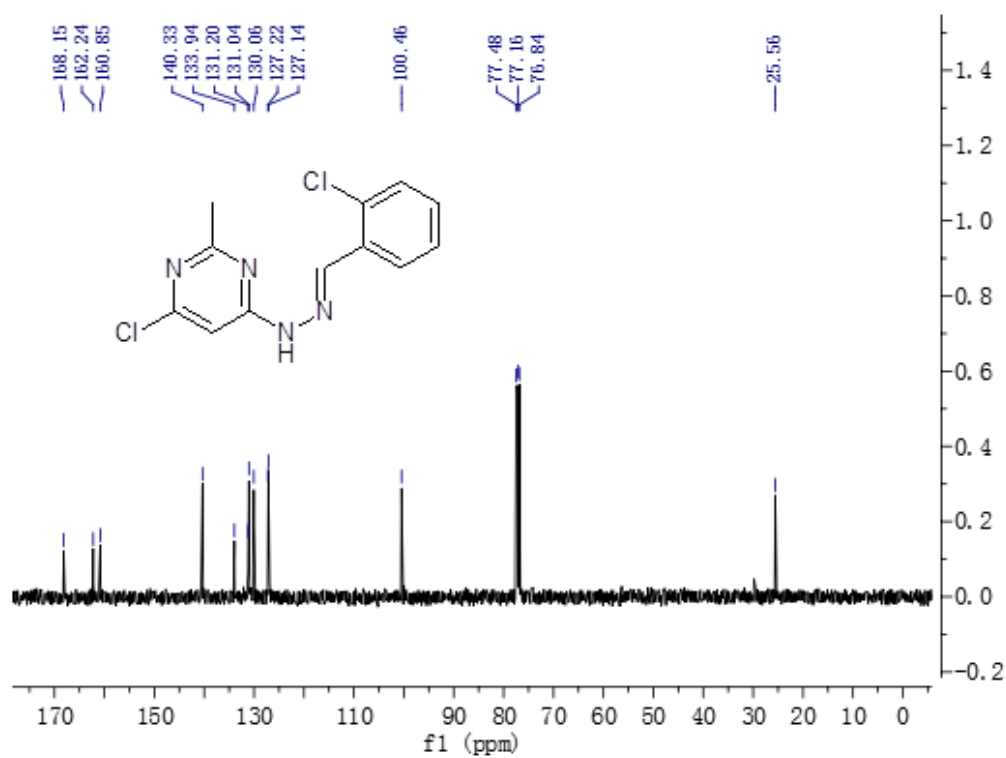
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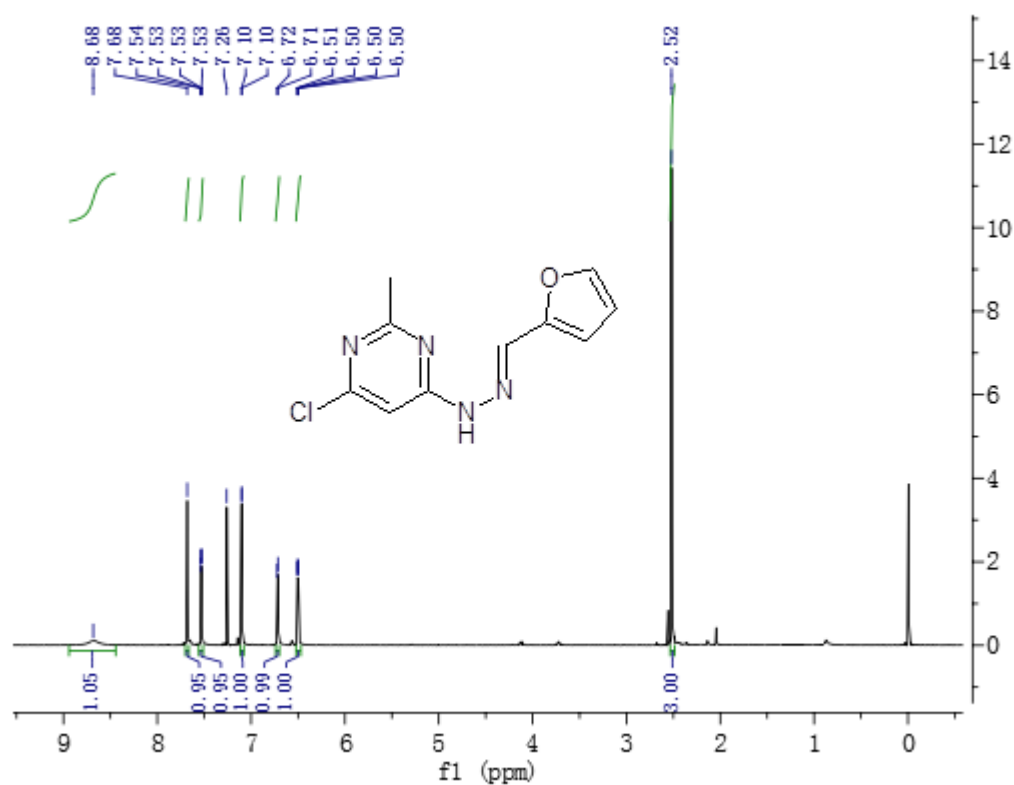
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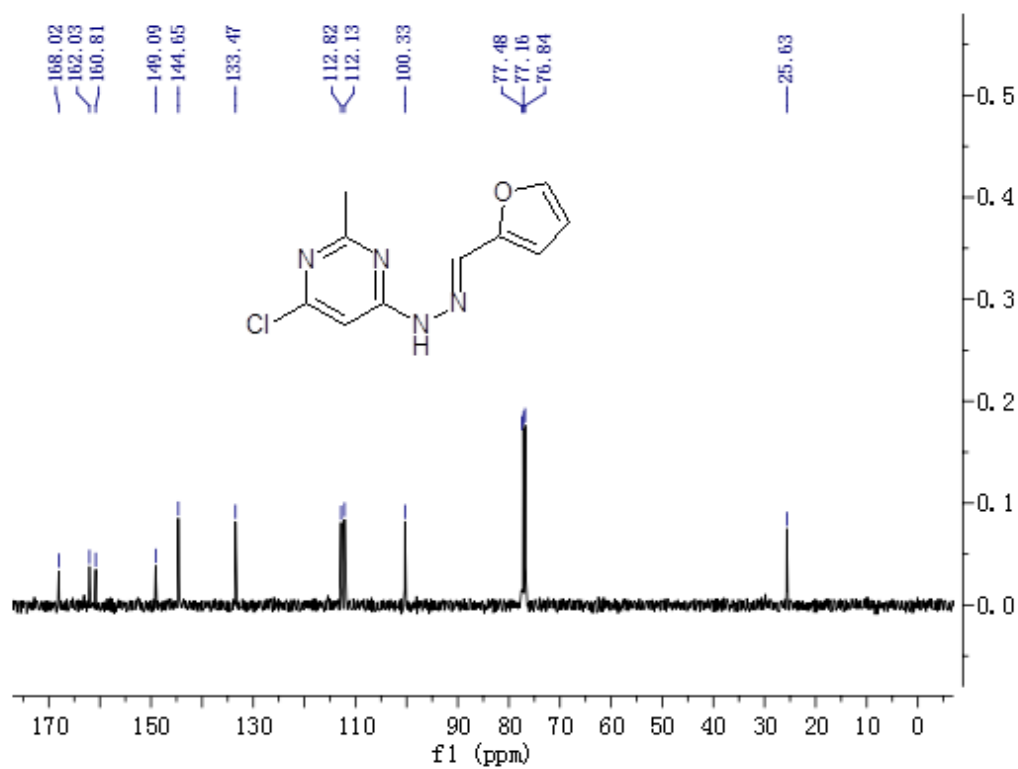
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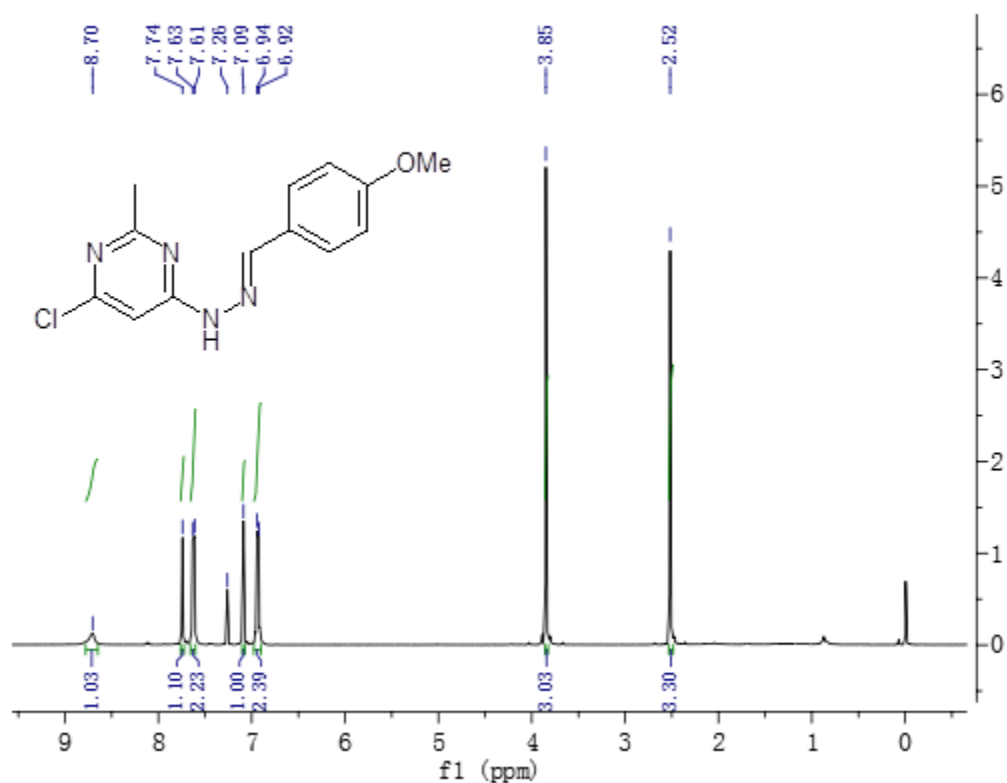
Furfural (6-chloro-2-methyl-4-pyrimidinyl)hydrazone (4h)



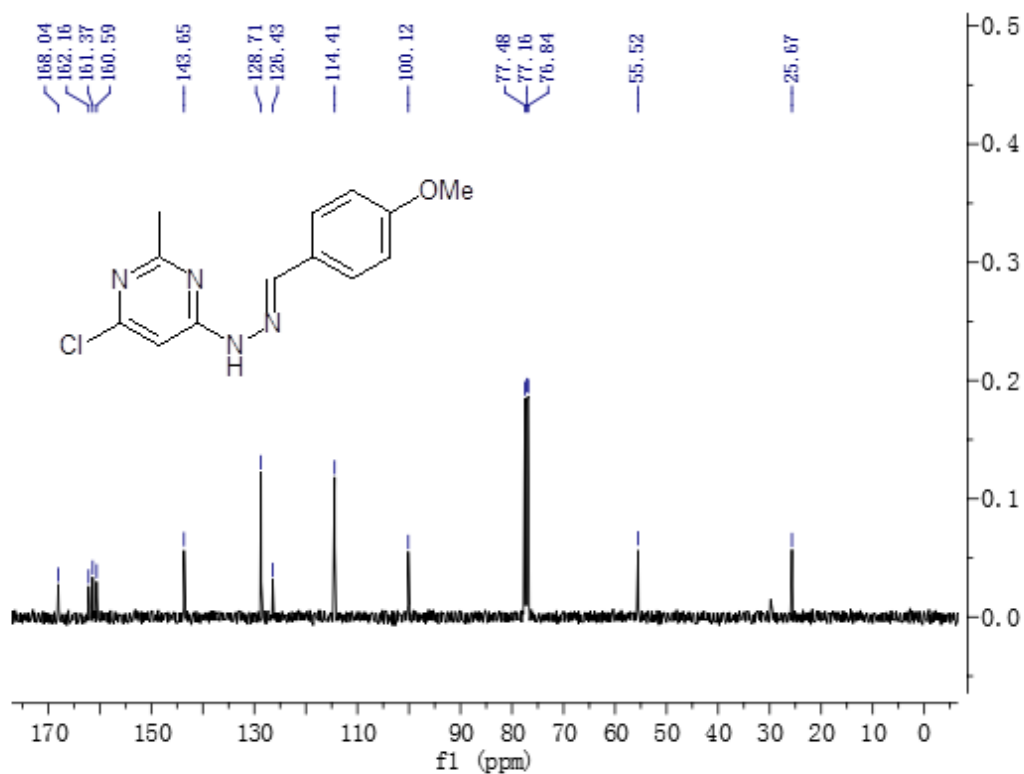
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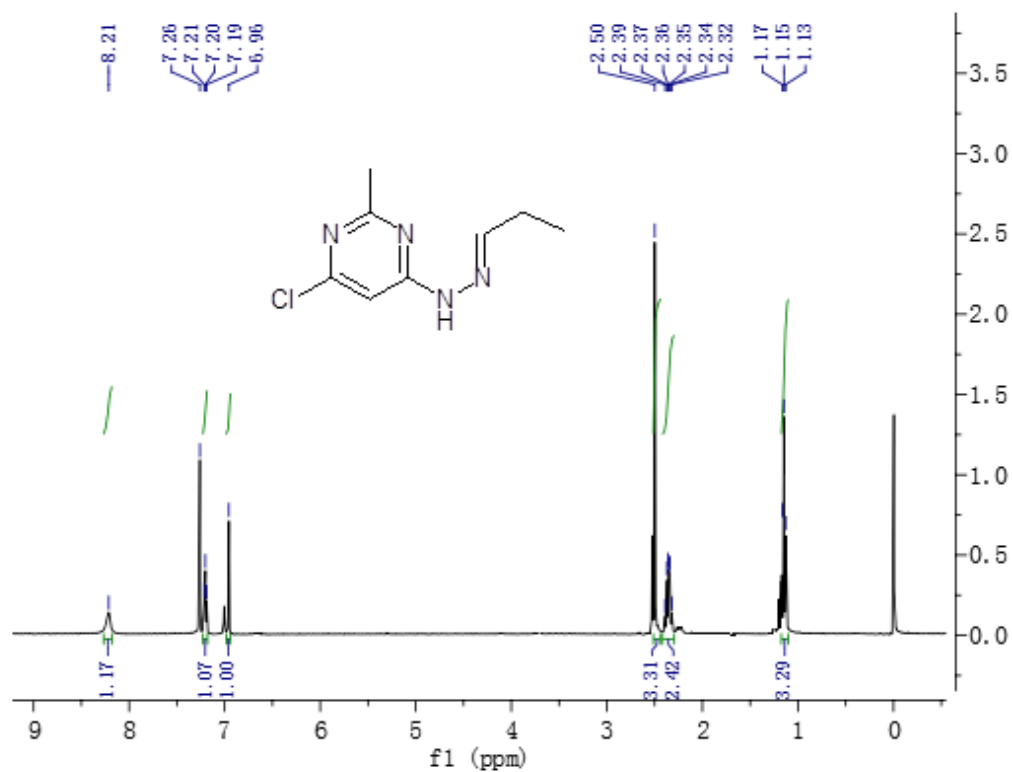
4-Methoxybenzaldehyde (6-chloro-2-methyl-4-pyrimidinyl)hydrazone (4i)



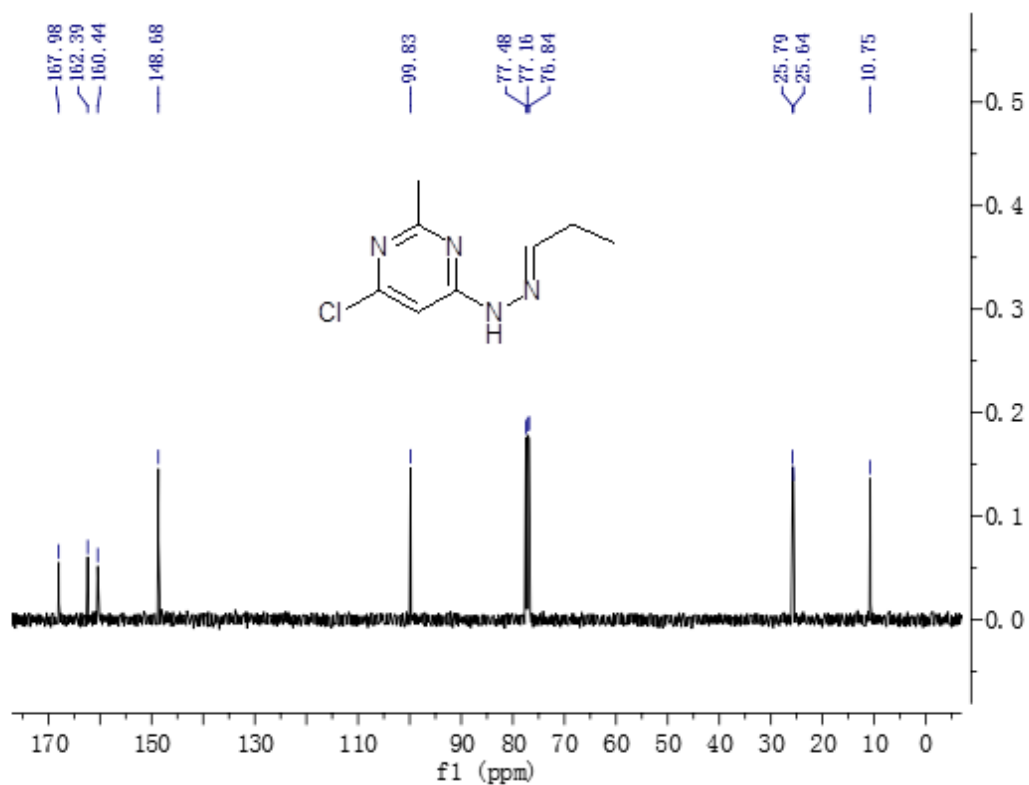
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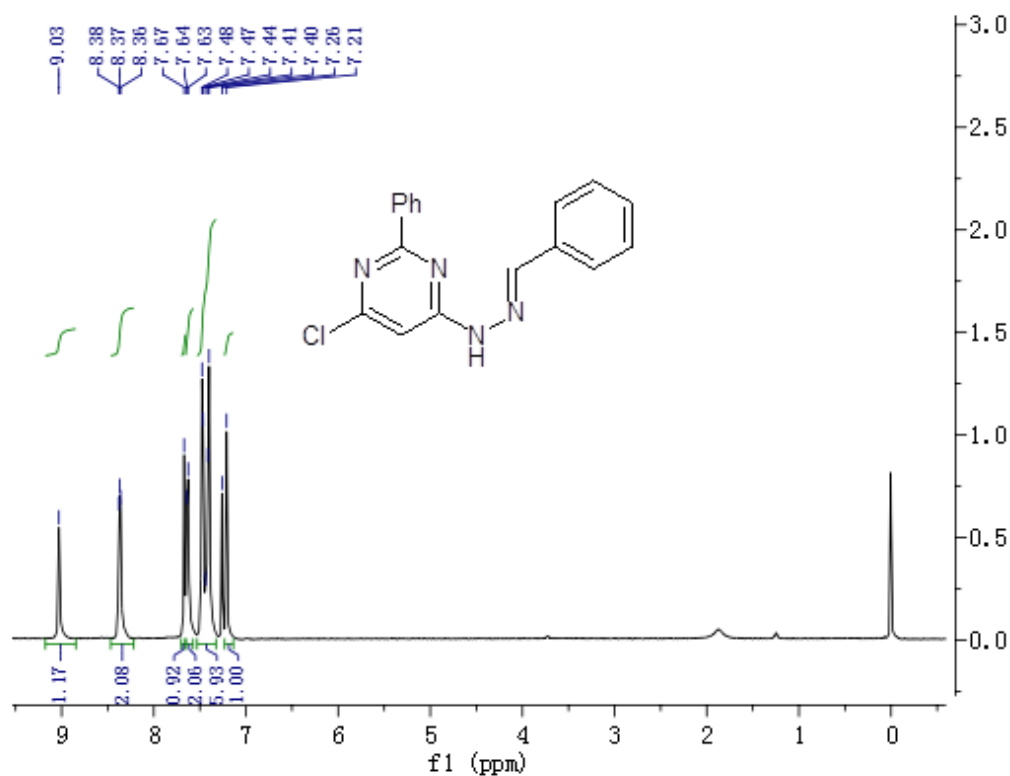
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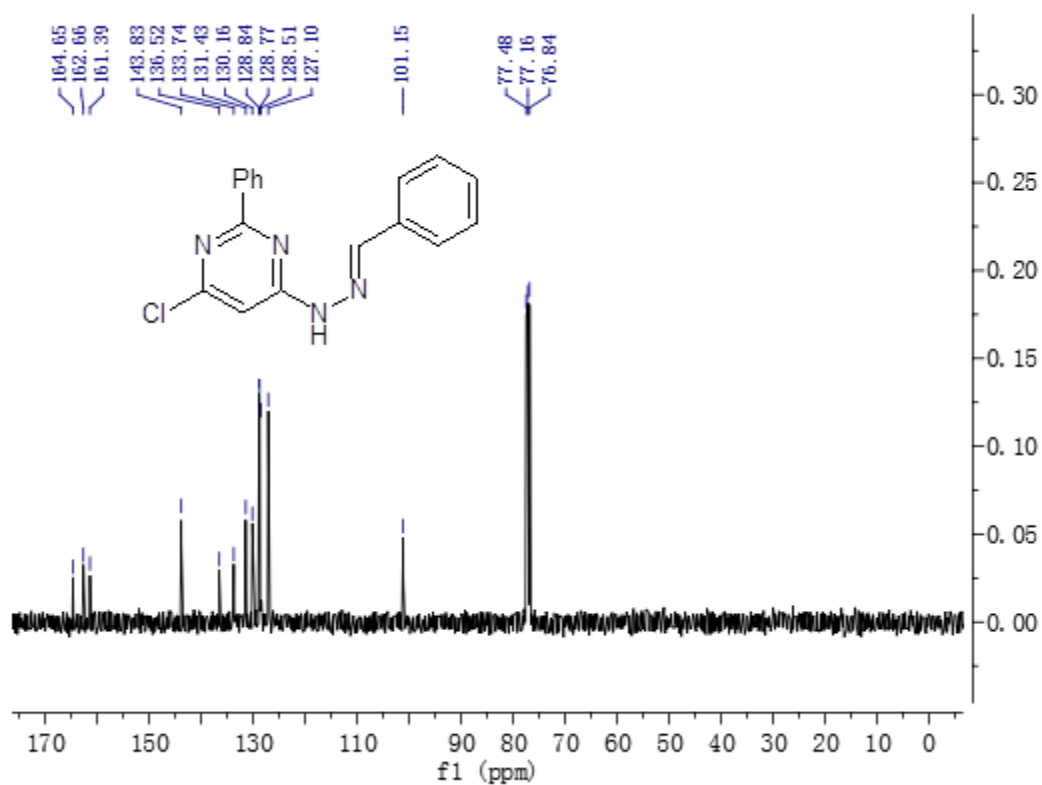
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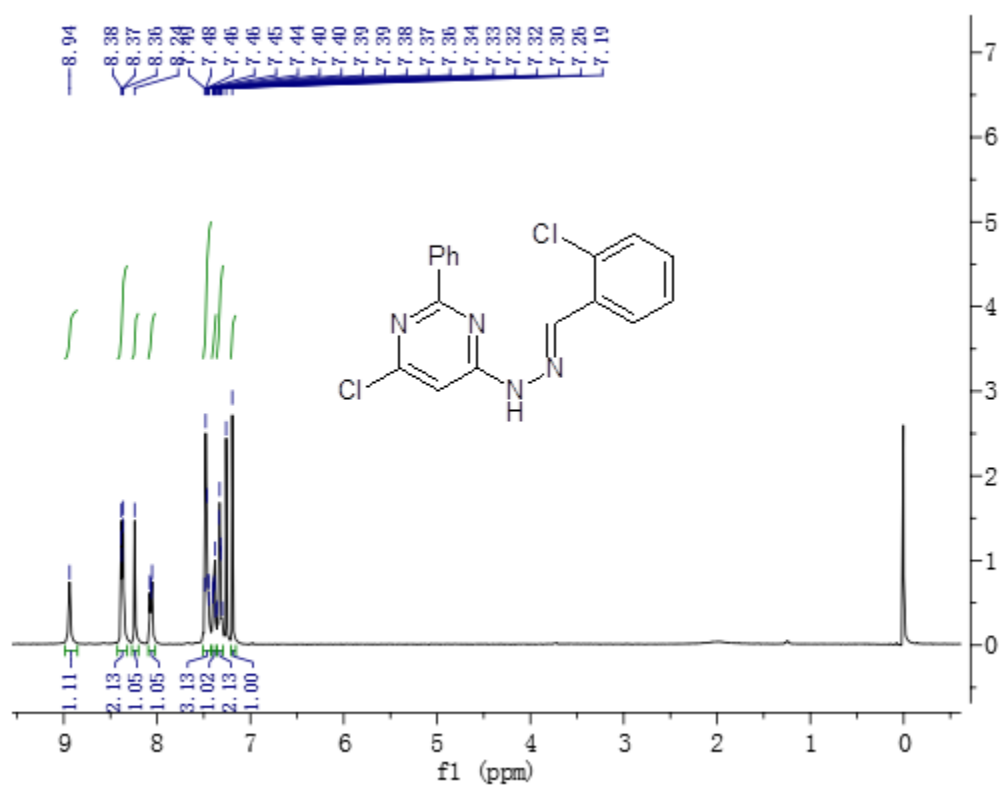
Benzaldehyde (6-chloro-2-phenyl-4-pyrimidinyl)hydrazone (4k)



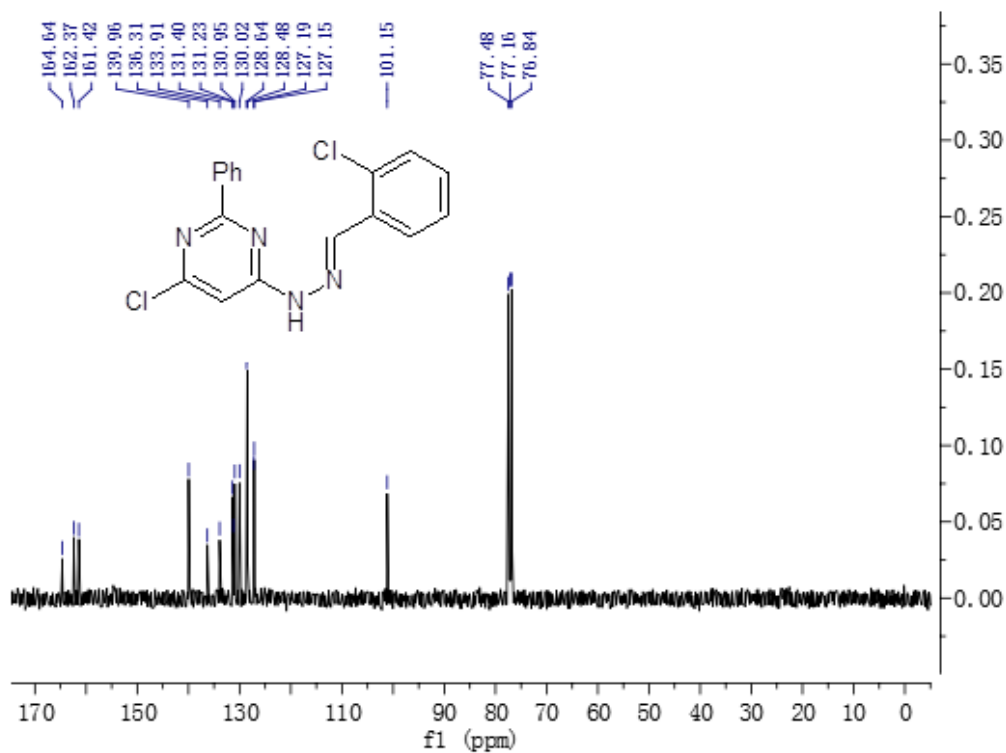
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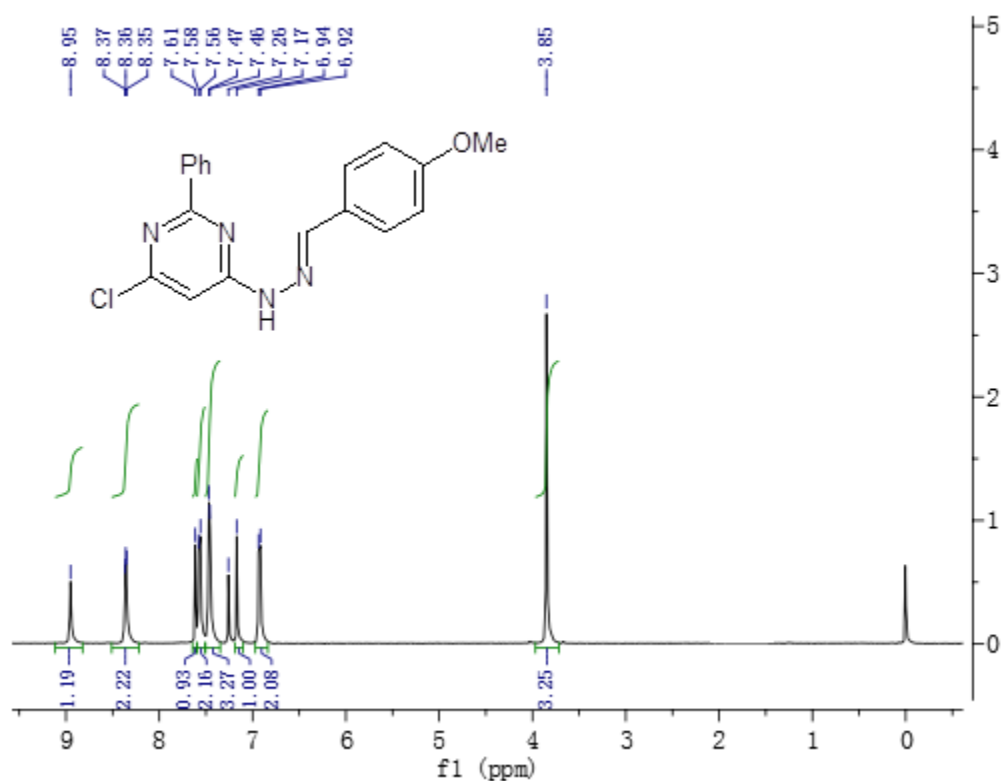
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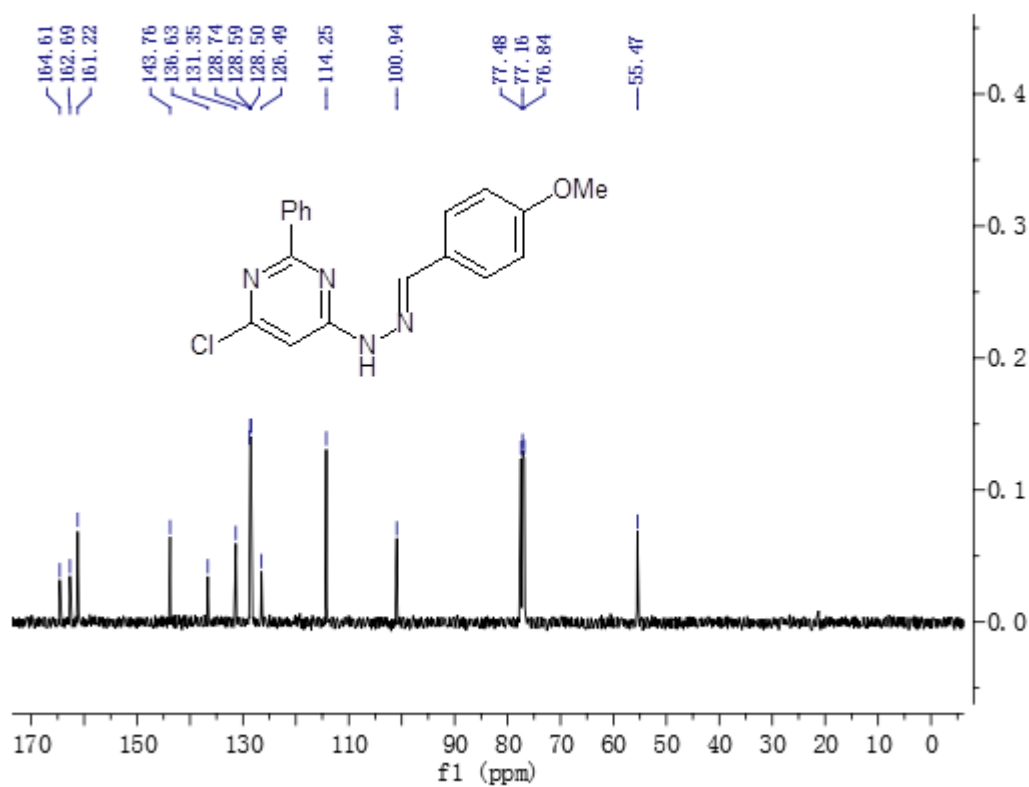
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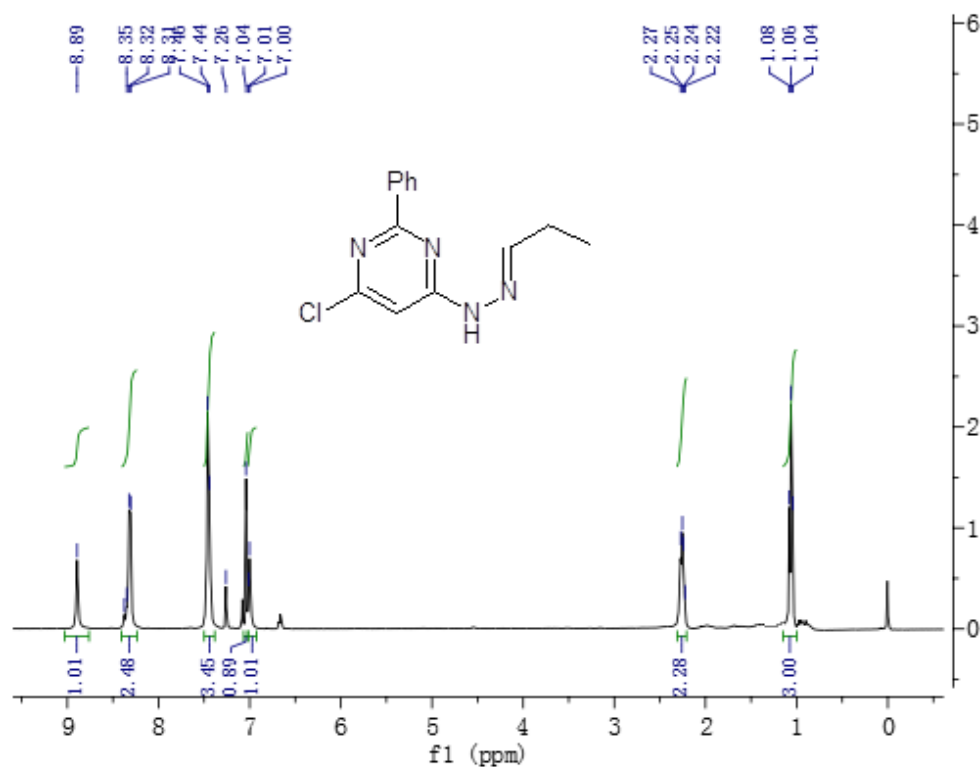
4-Methoxybenzaldehyde (6-chloro-2-phenyl-4-pyrimidinyl)hydrazone (4n)



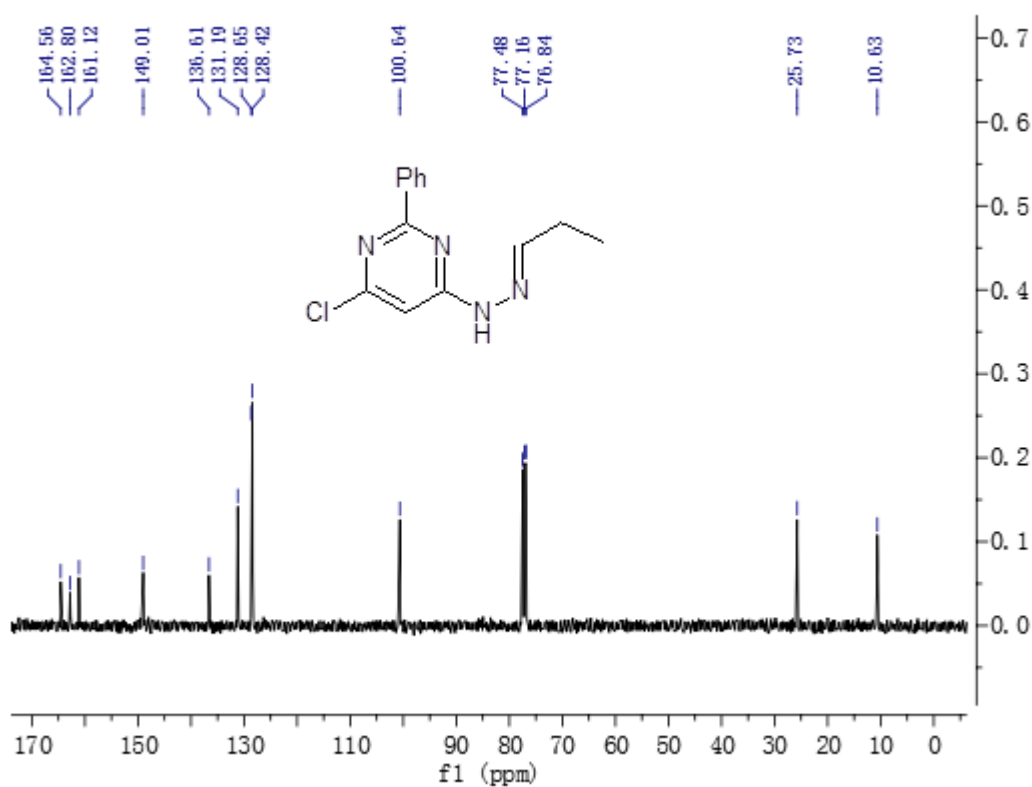
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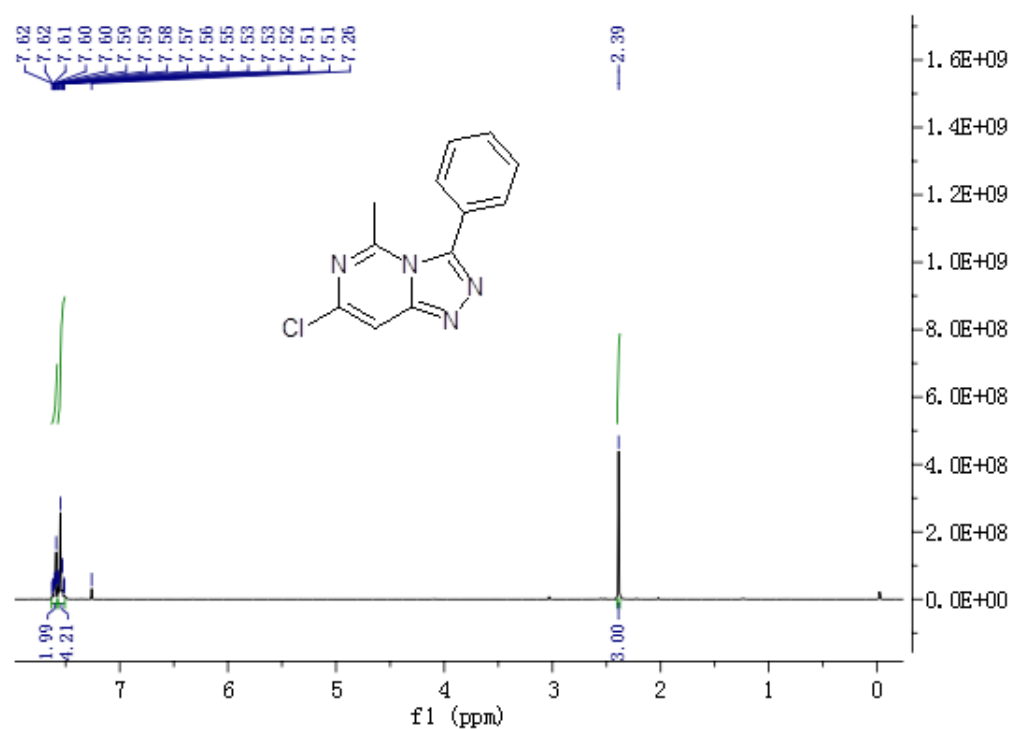
Propanaldehyde (6-chloro-2-phenyl-4-pyrimidinyl)hydrazone (4o)



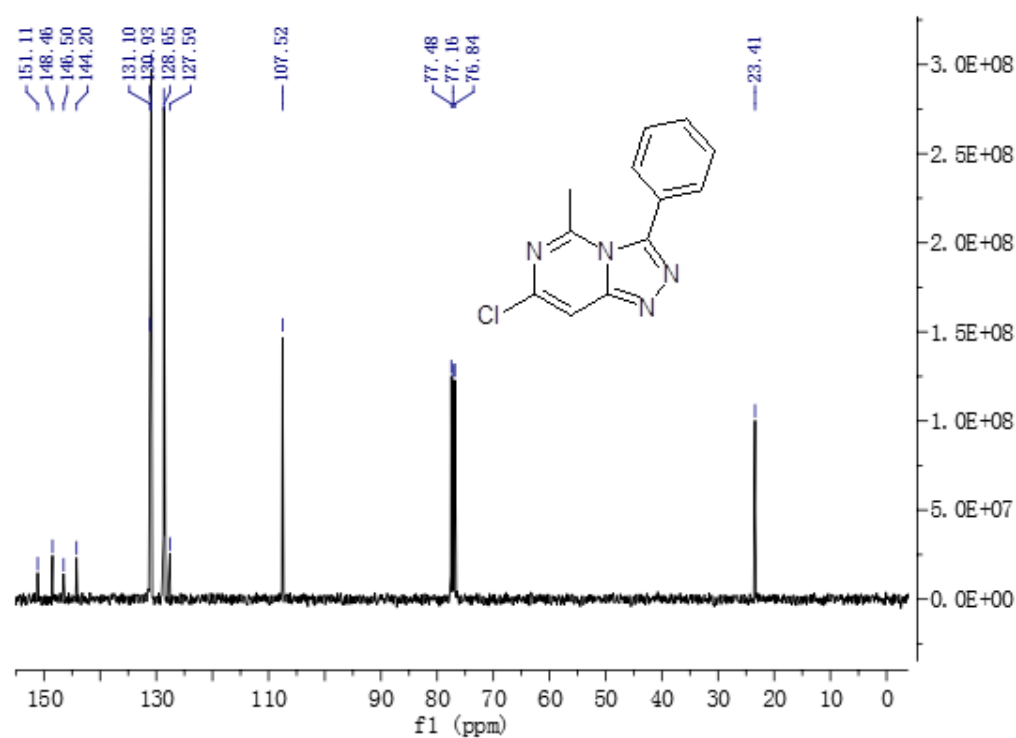
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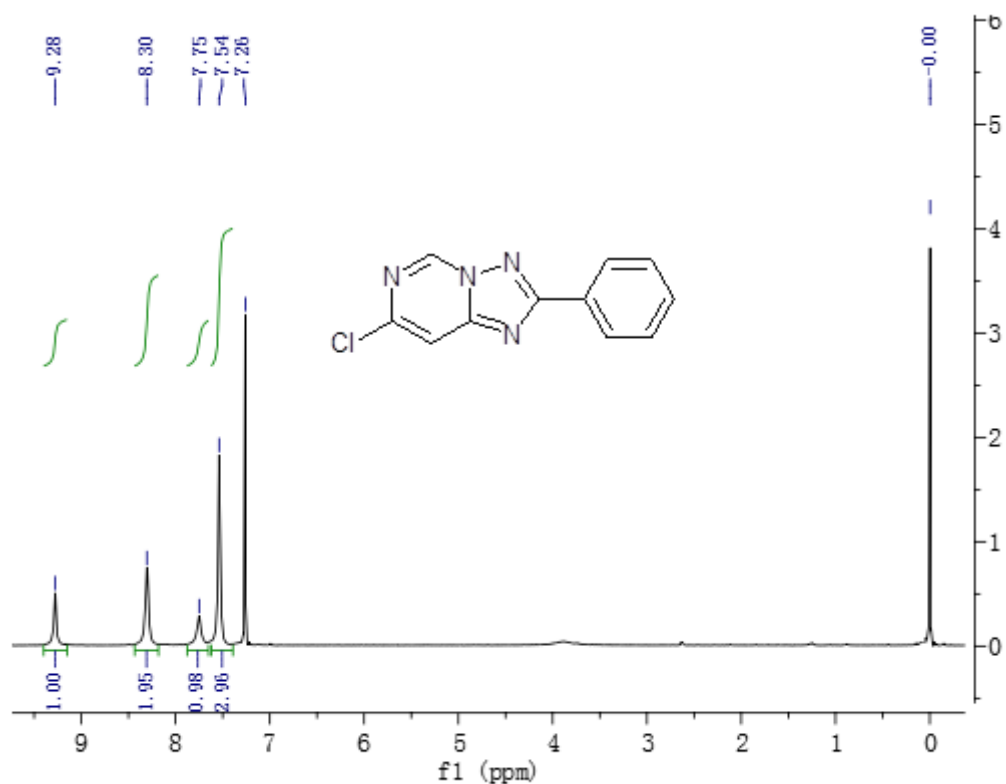
Spectra of 7-chloro-5-methyl-3-phenyl-[1,2,4]triazolo[4,3-c]pyrimidine (5f)



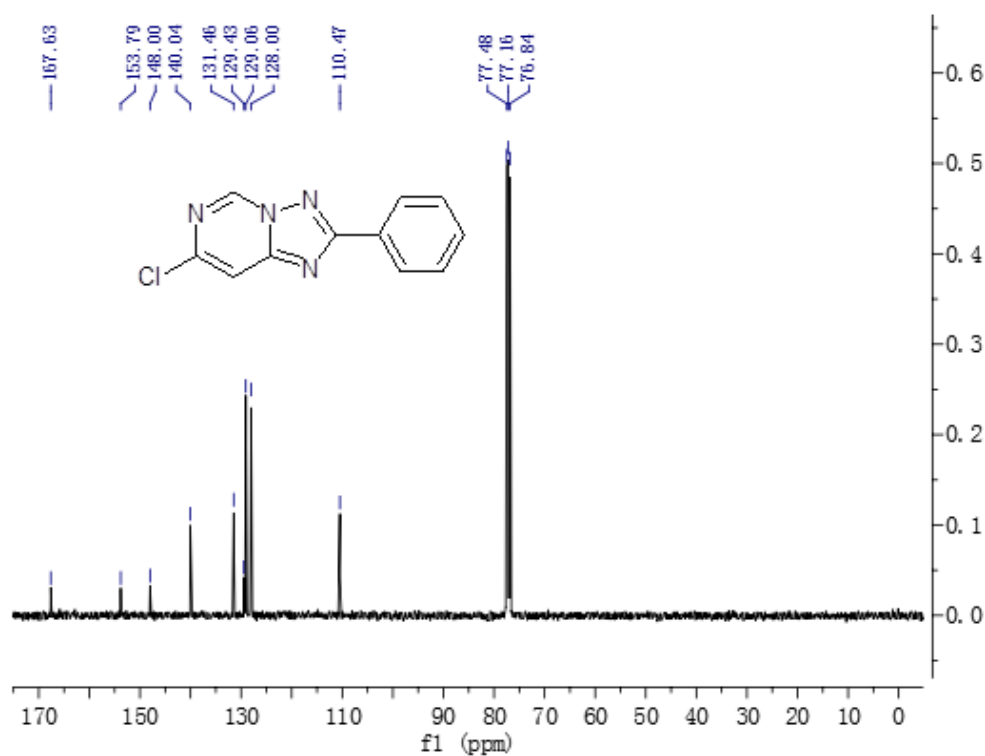
7-Chloro-5-methyl-3-phenyl-[1,2,4]triazolo[4,3-c]pyrimidine (5f)



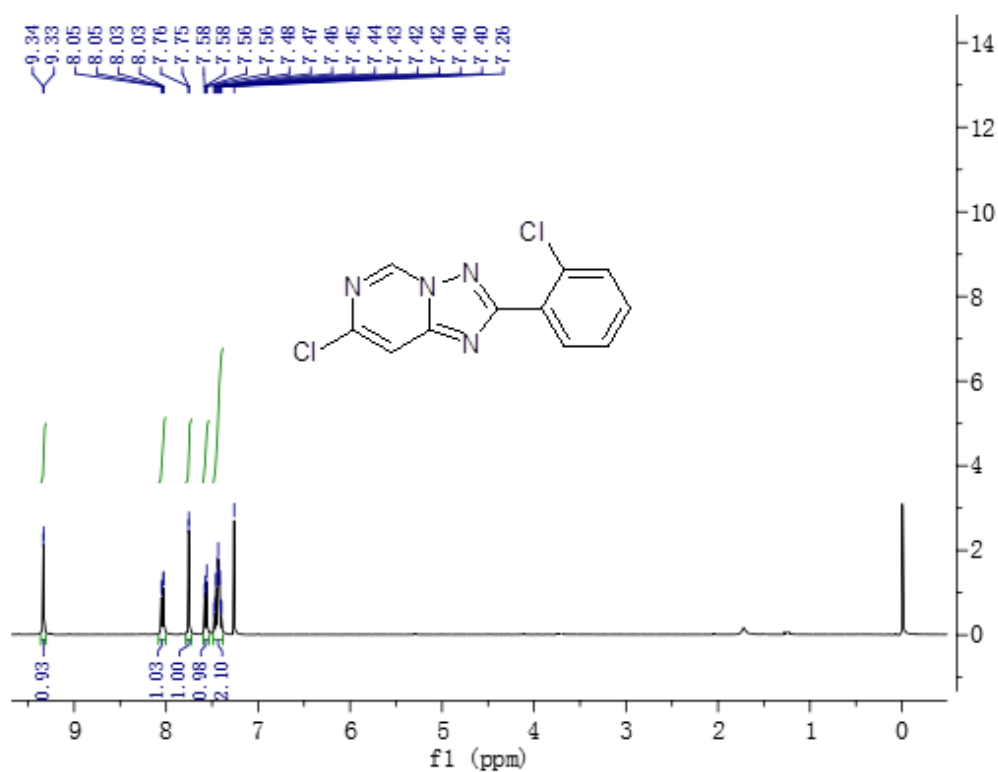
Spectra of 7-chloro-[1,2,4]triazolo[1,5-c]pyrimidines 6
7-Chloro-2-phenyl-[1,2,4]triazolo[1,5-c]pyrimidine (6a)



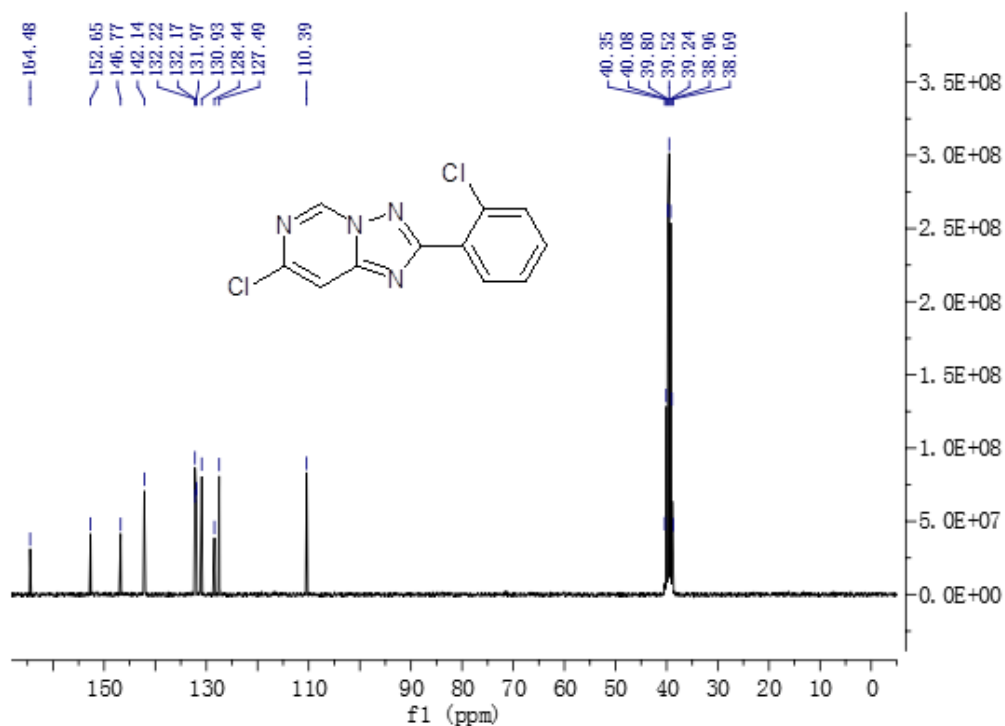
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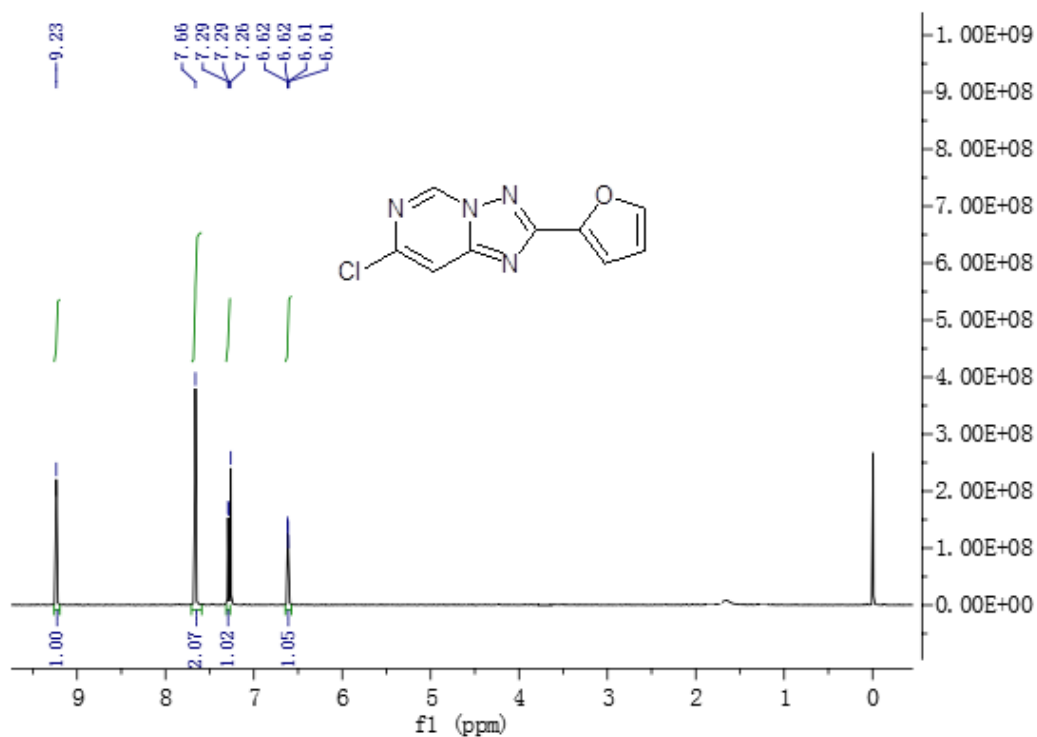
7-Chloro-2-(2-chlorophenyl)-[1,2,4]triazolo[1,5-c]pyrimidine (6b)



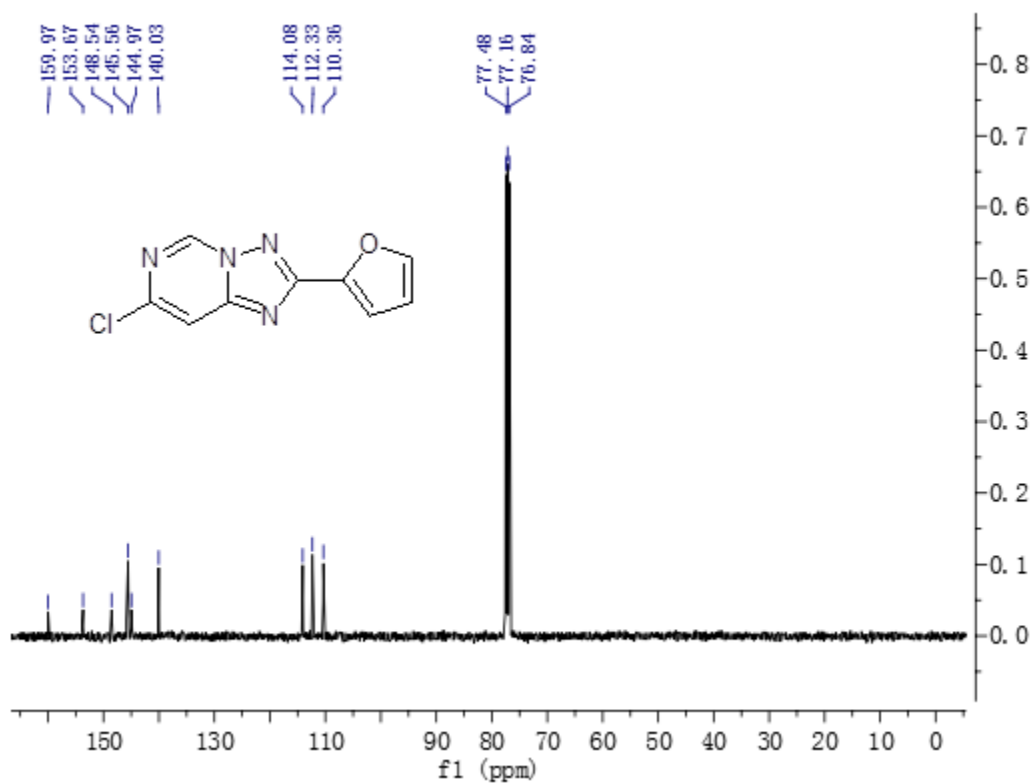
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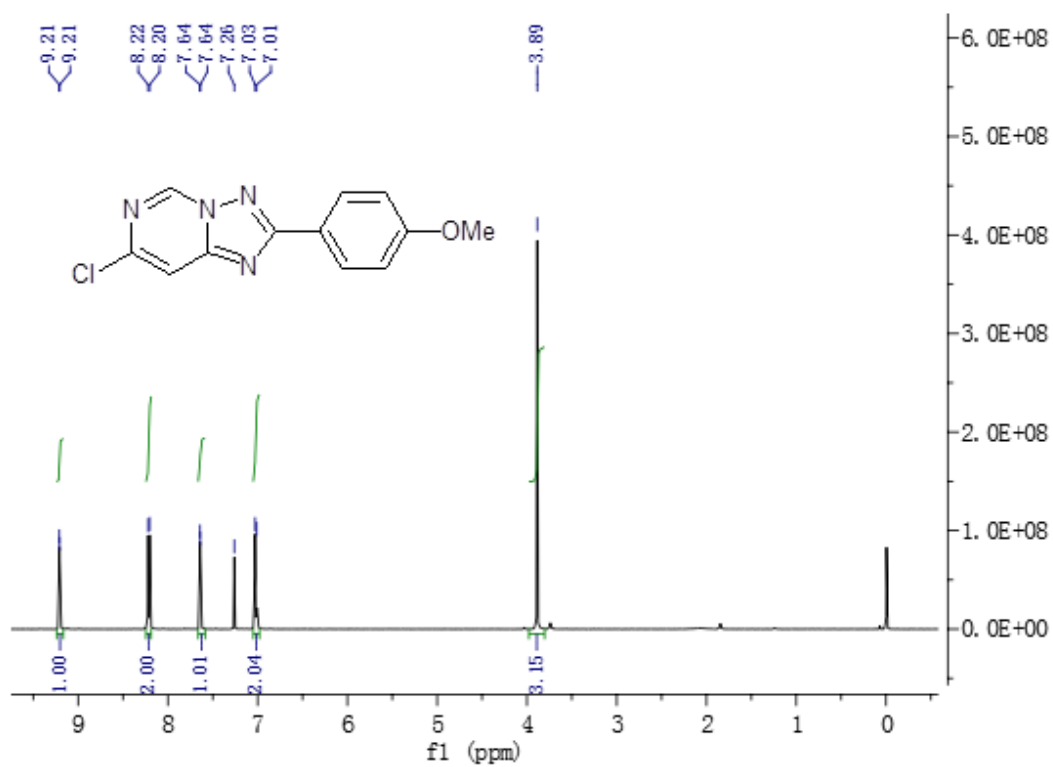
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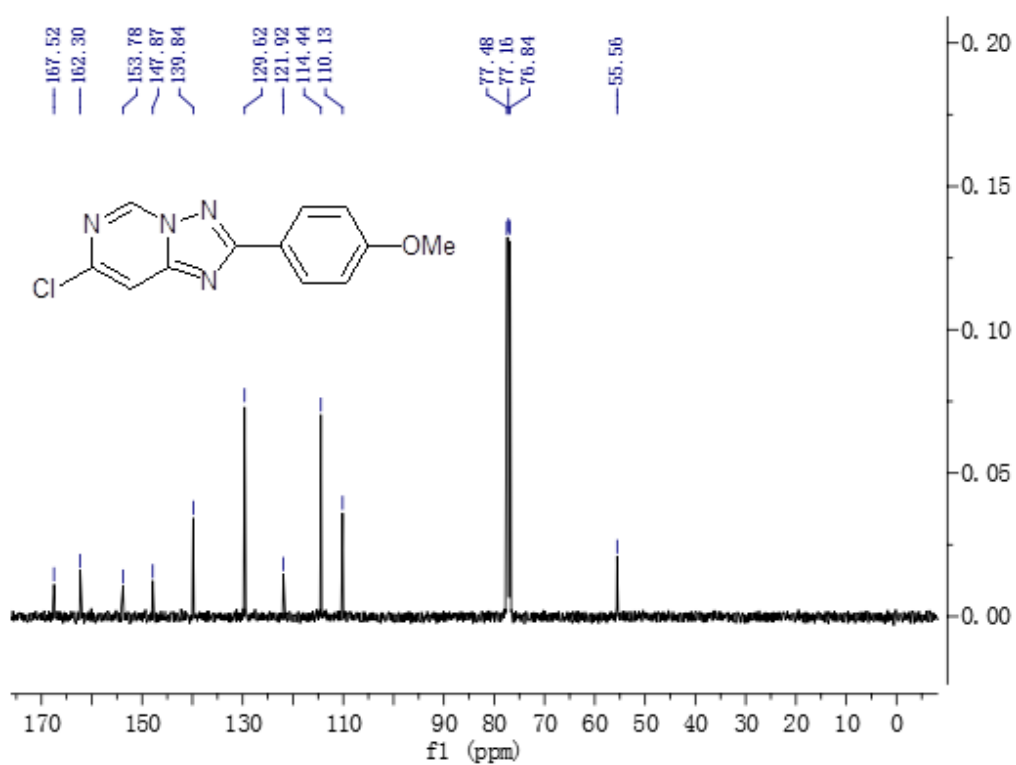
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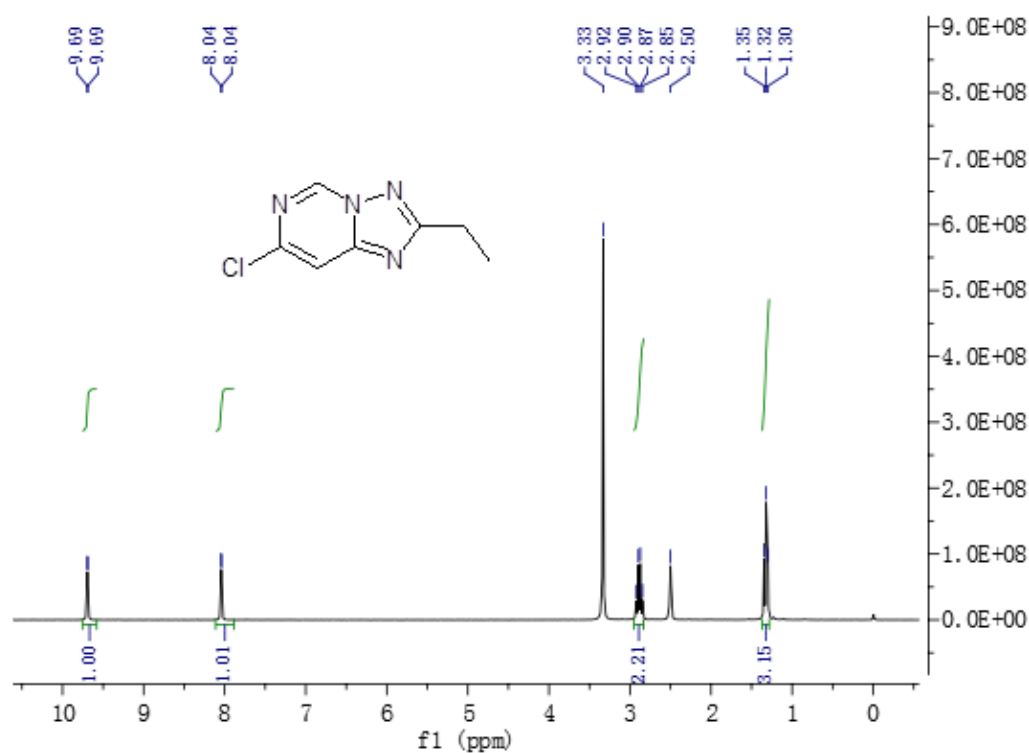
7-Chloro-2-(4-methoxyphenyl)-[1,2,4]triazolo[1,5-c]pyrimidine (6d)



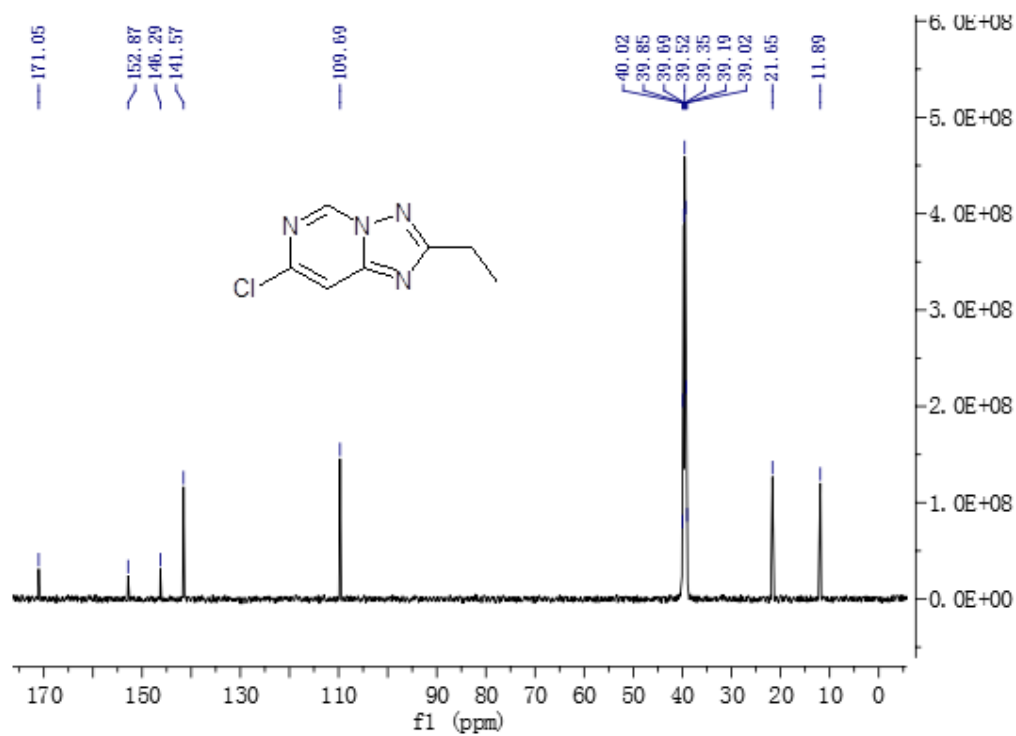
7-Chloro-2-(4-methoxyphenyl)-[1,2,4]triazolo[1,5-c]pyrimidine (6d)



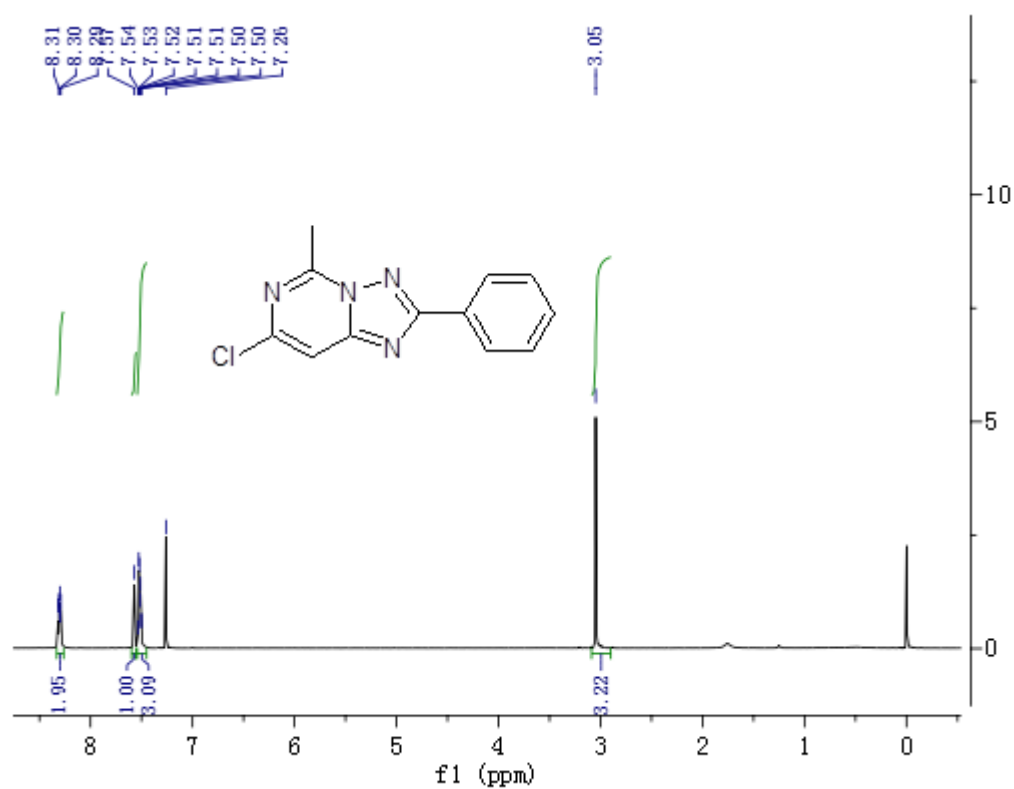
7-Chloro-2-ethyl-[1,2,4]triazolo[1,5-c]pyrimidine (6e)



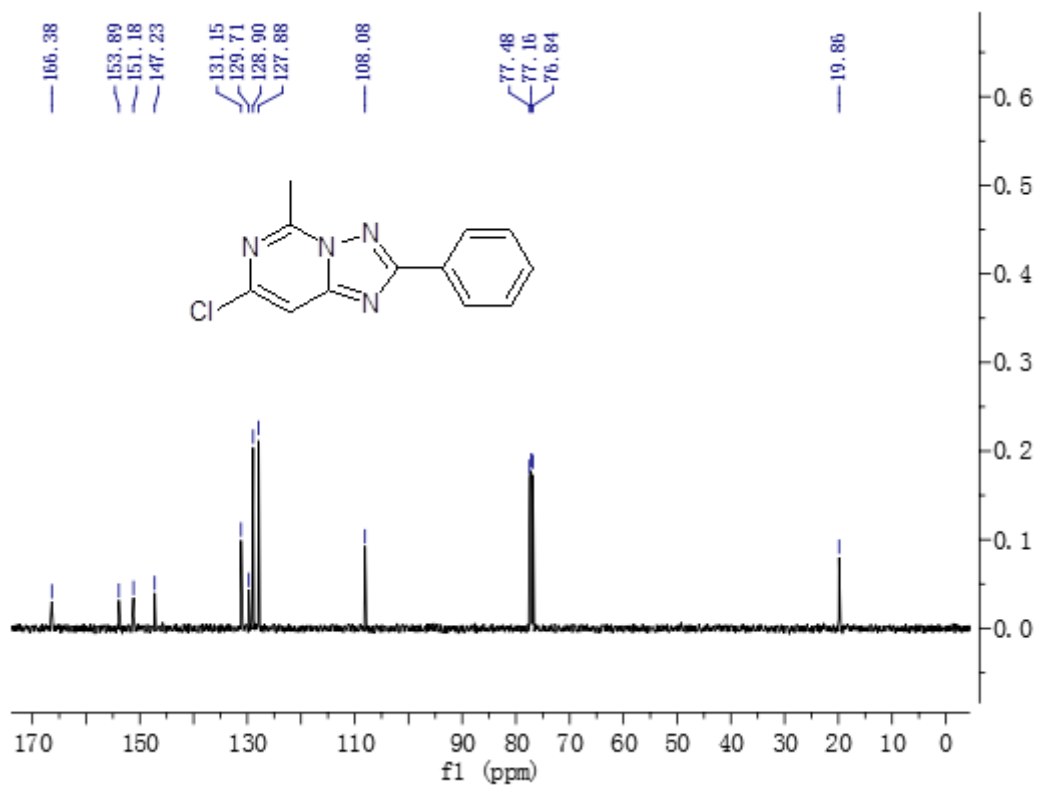
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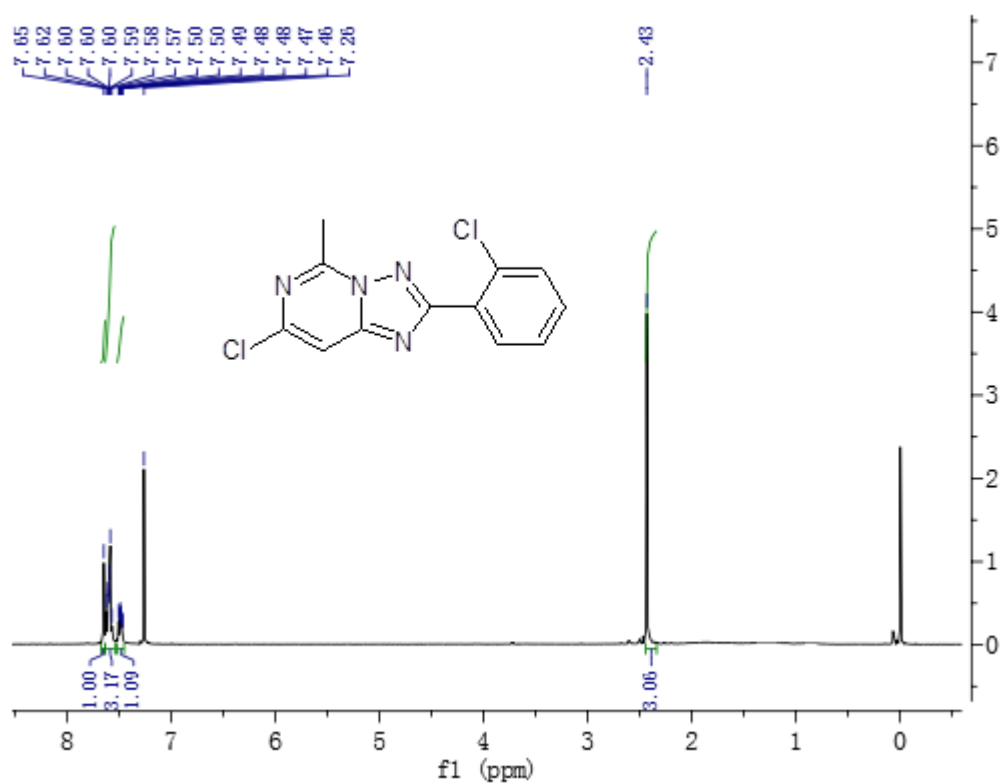
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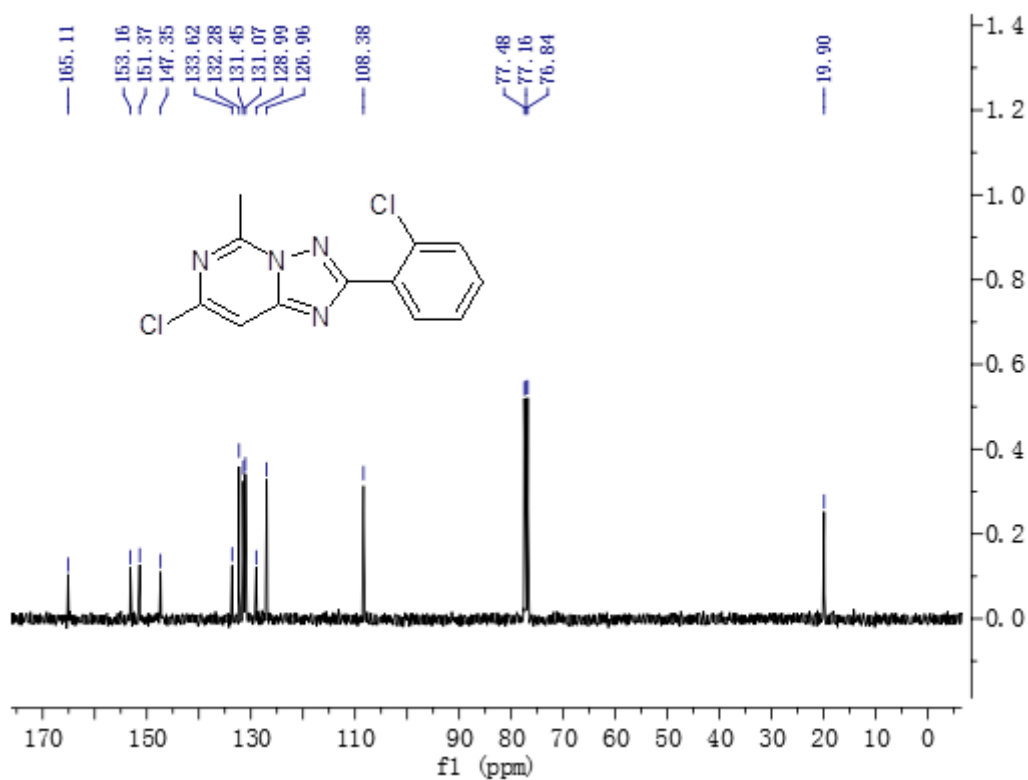
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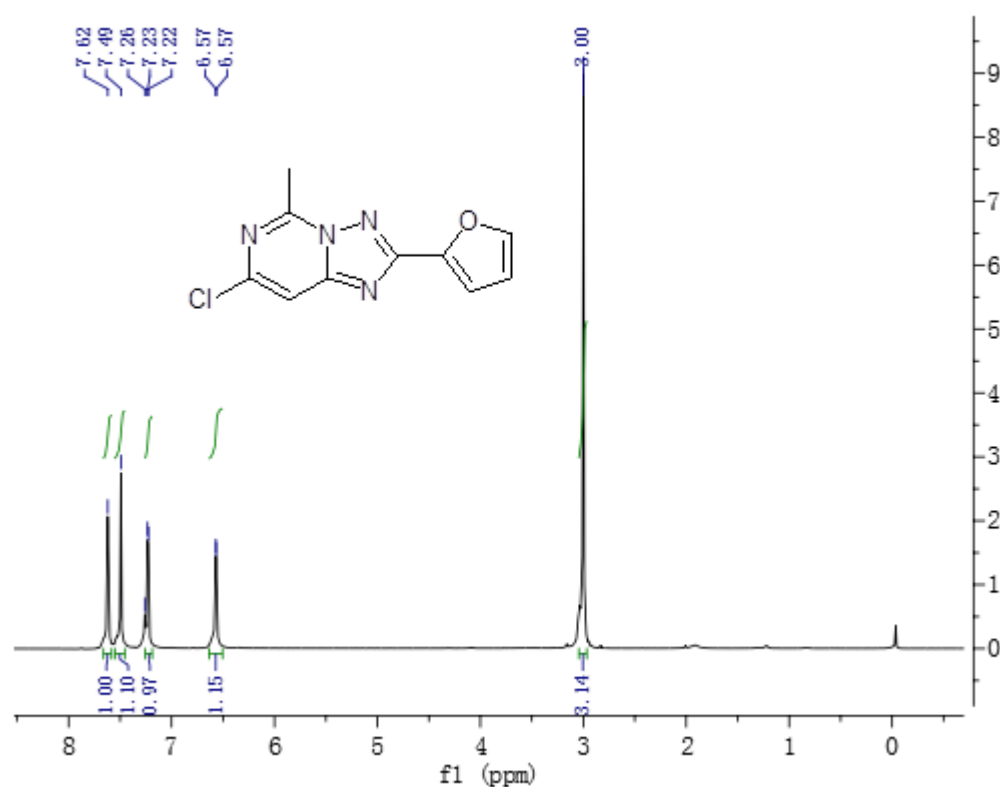
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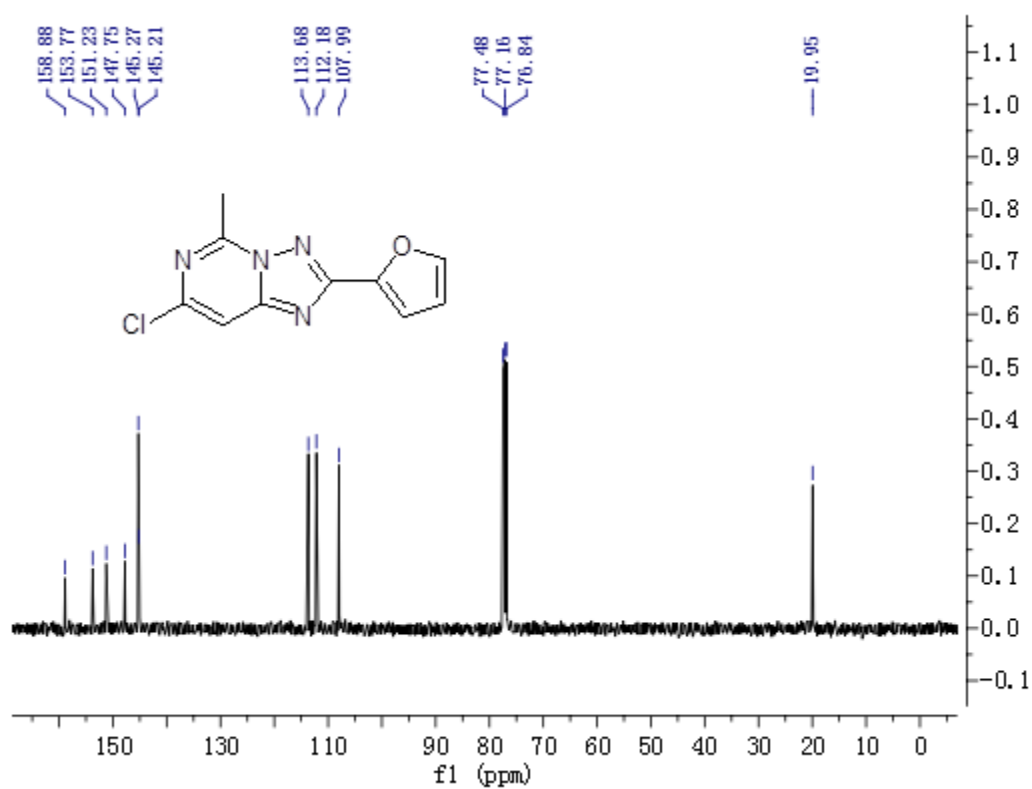
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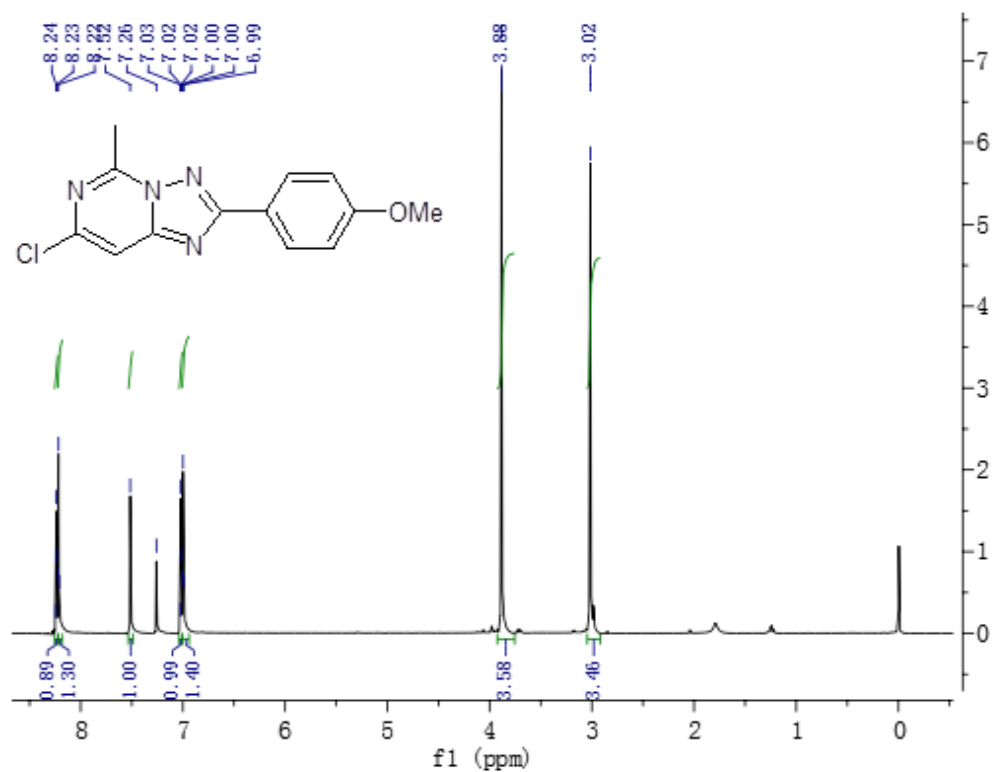
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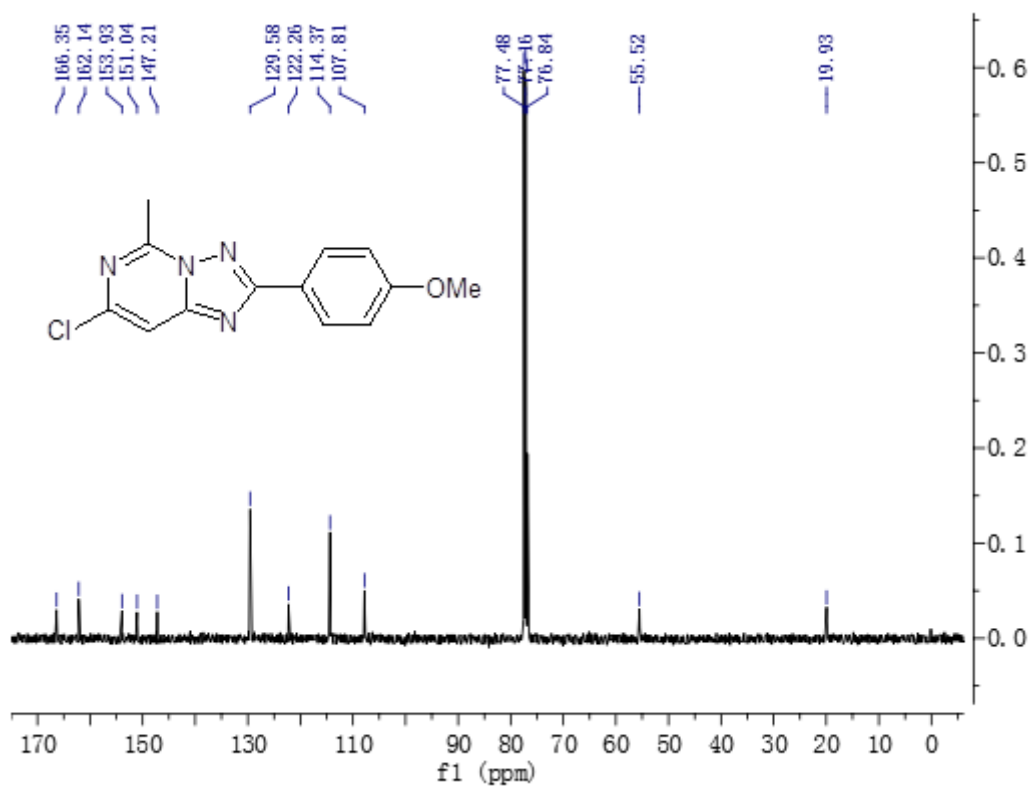
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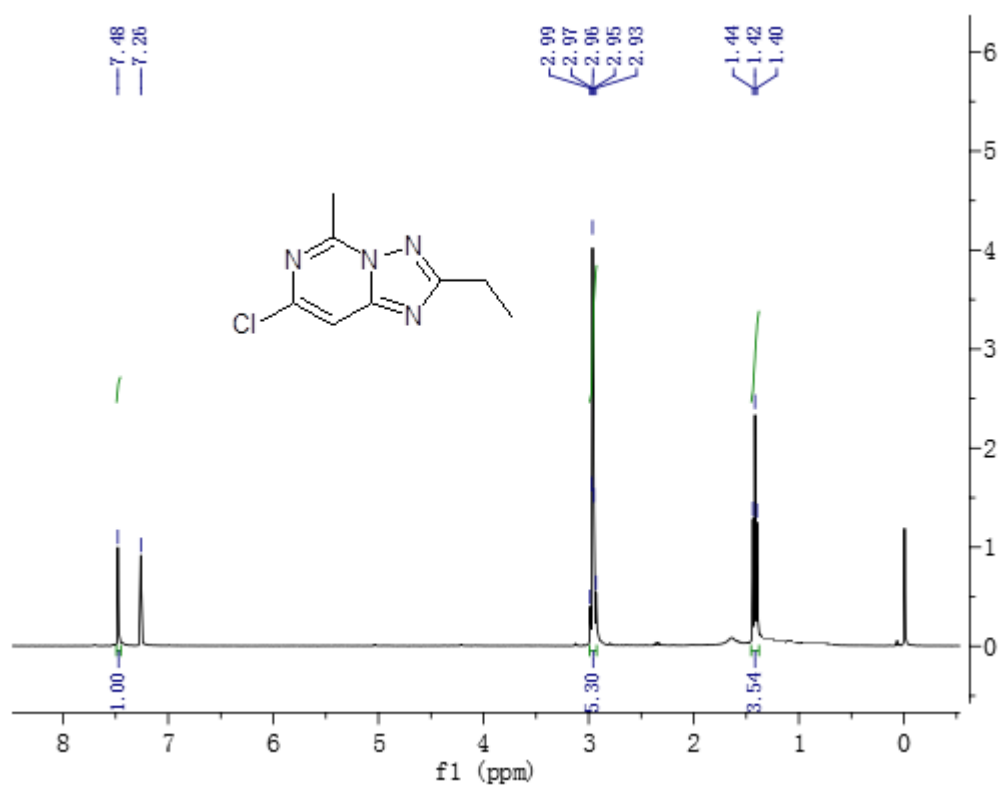
7-Chloro-2-(4-methoxyphenyl)-5-methyl-[1,2,4]triazolo[1,5-c]pyrimidine (6i)



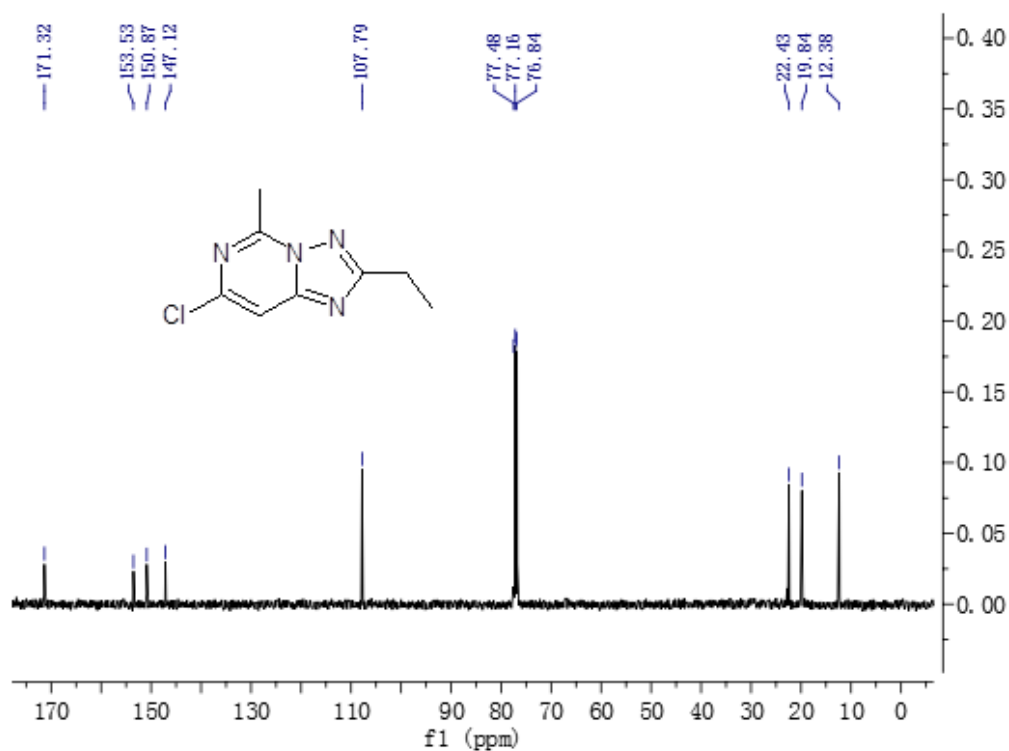
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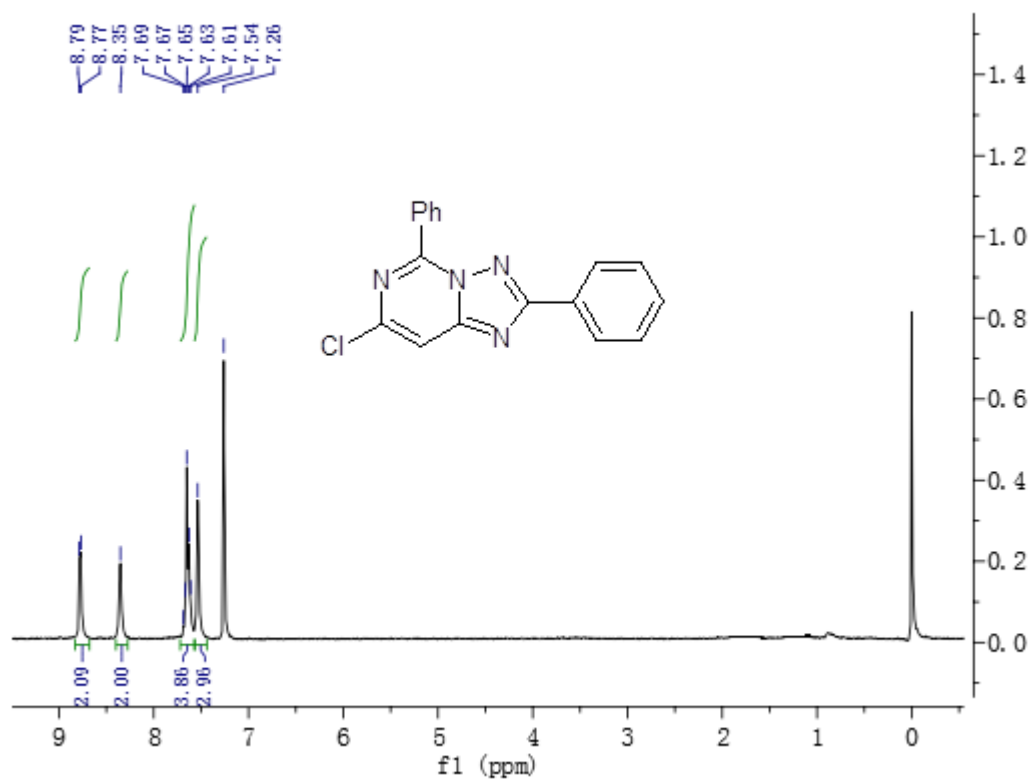
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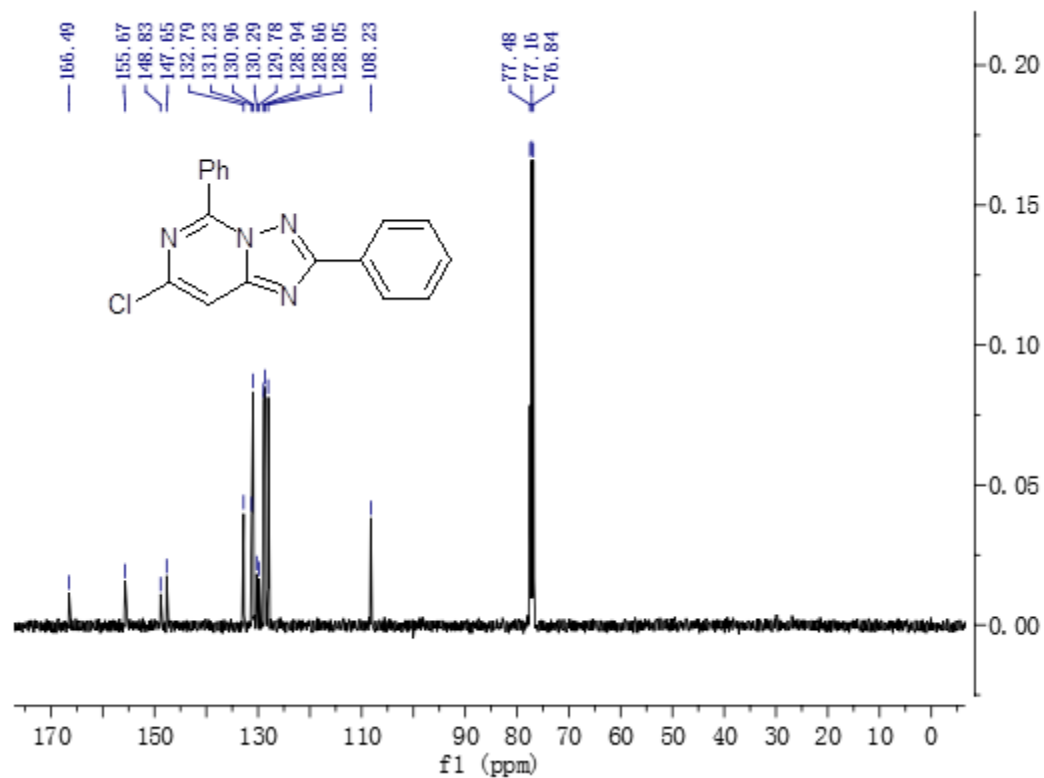
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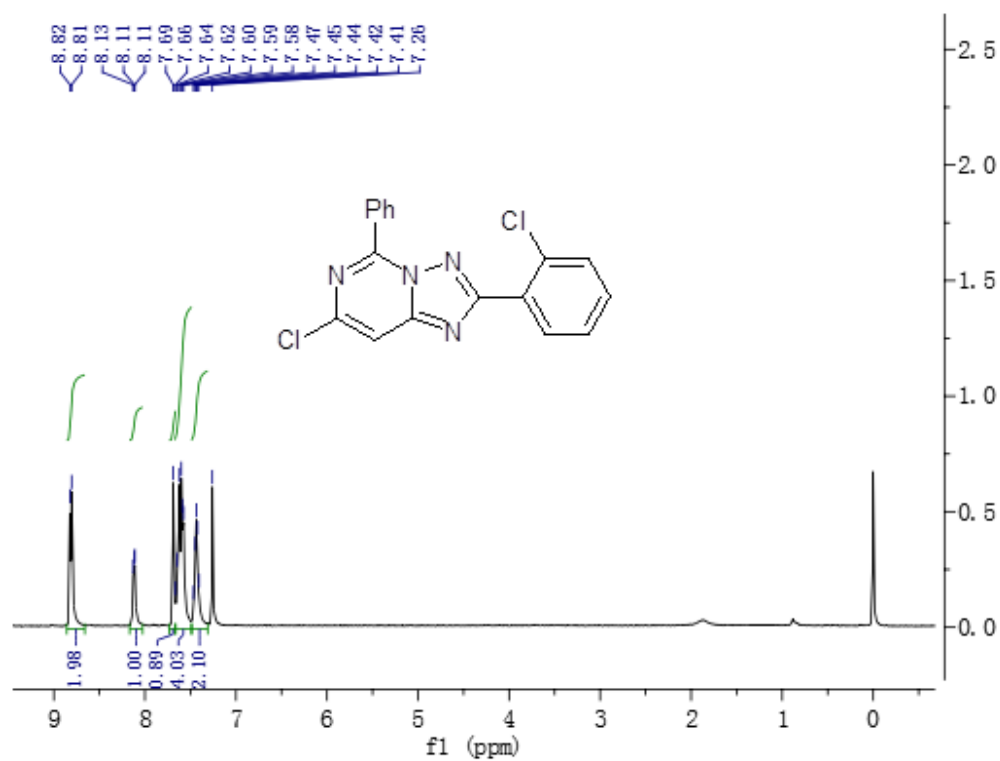
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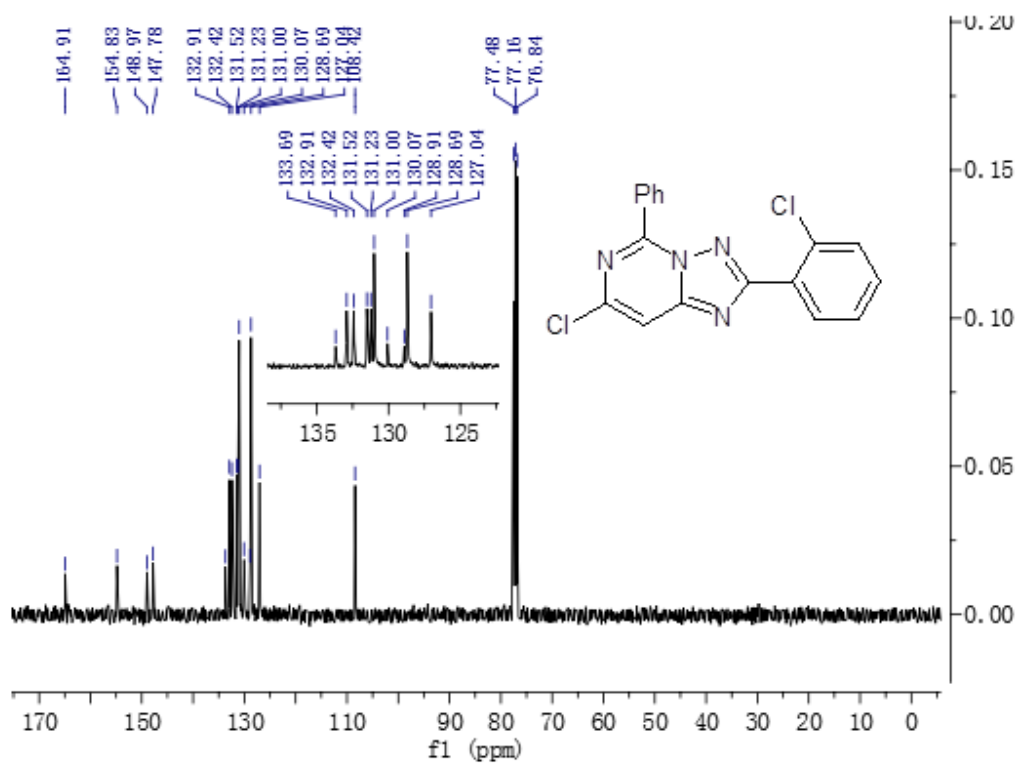
7-Chloro-2,5-diphenyl-[1,2,4]triazolo[1,5-c]pyrimidine (6k)



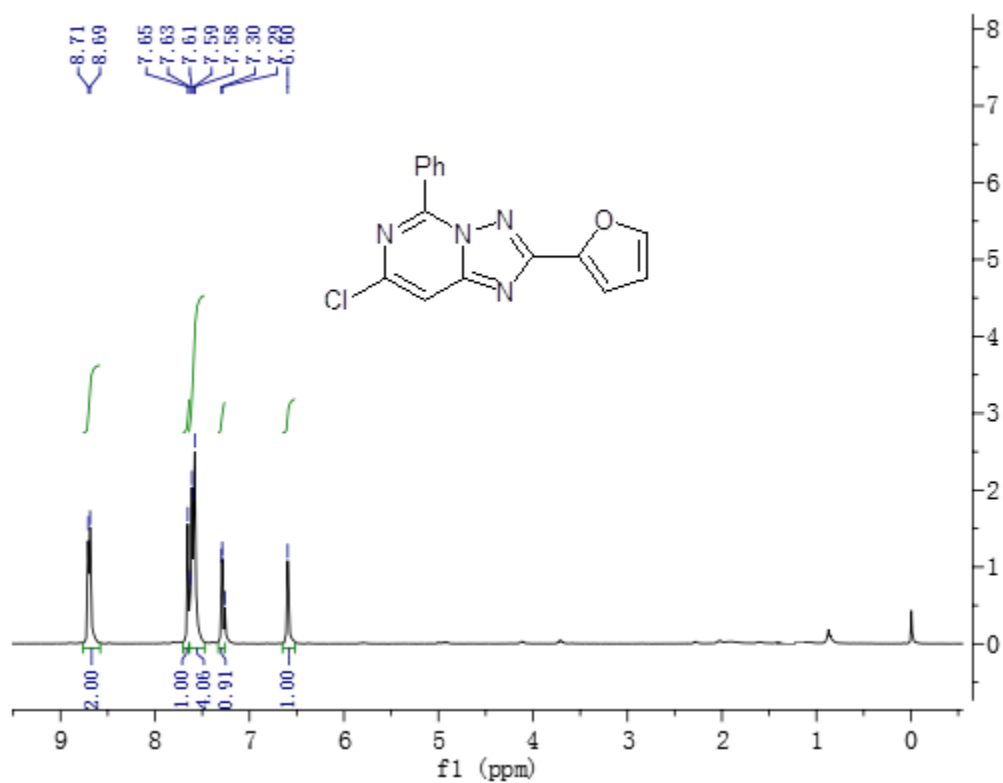
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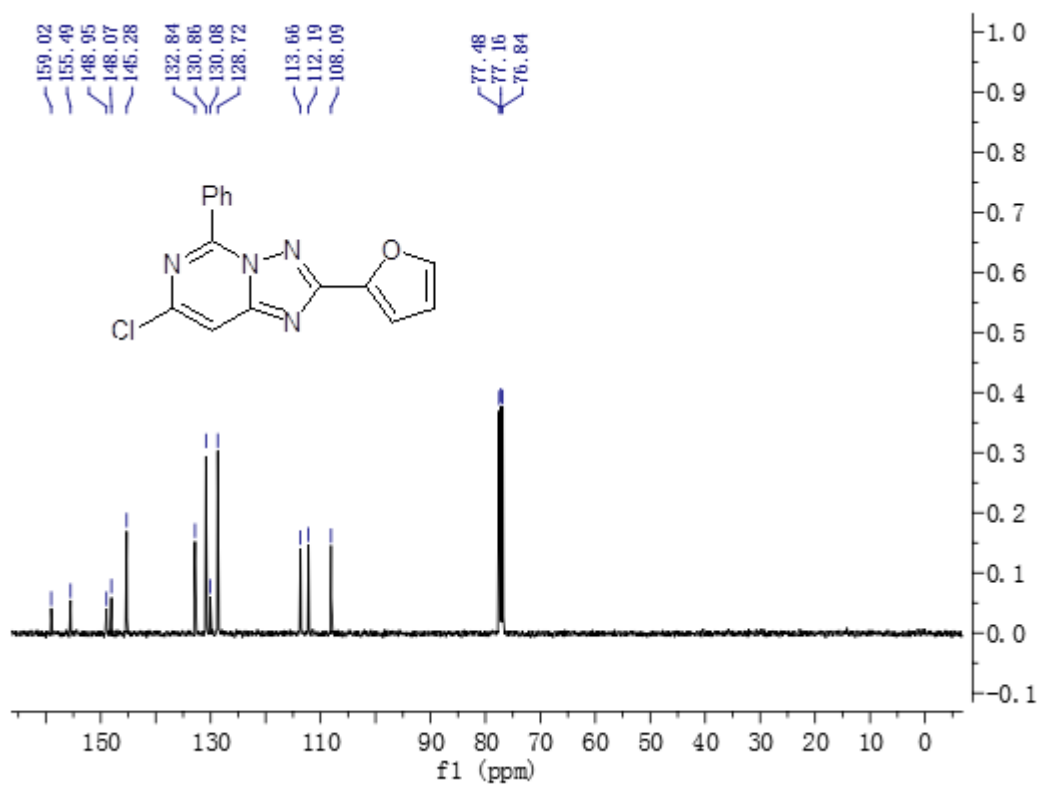
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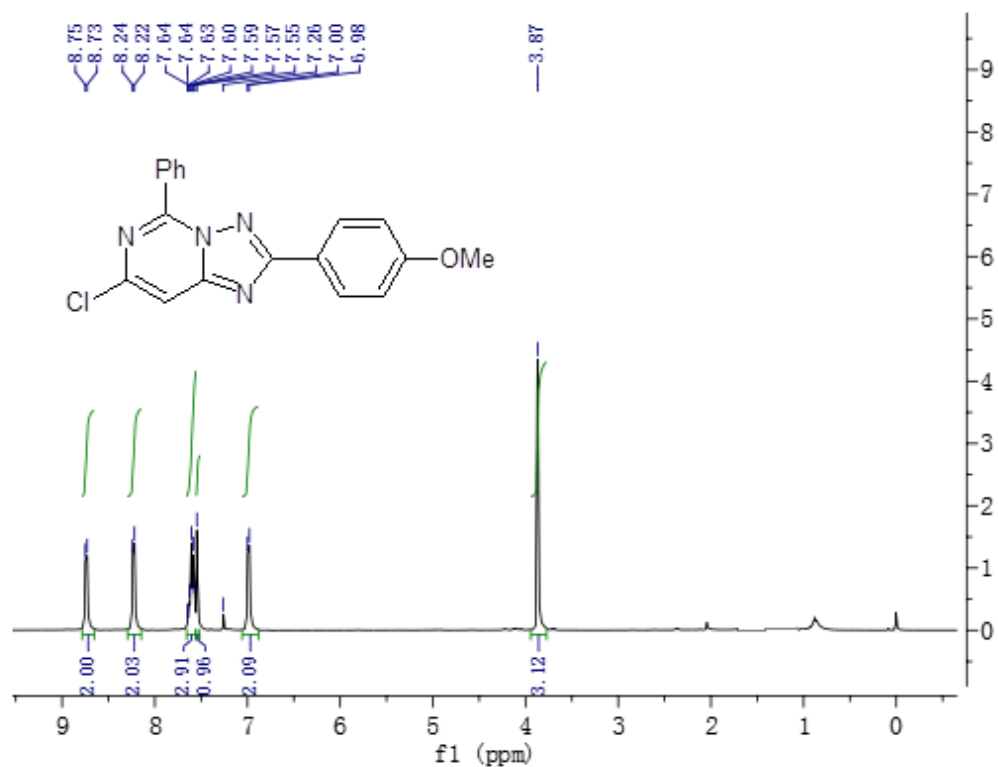
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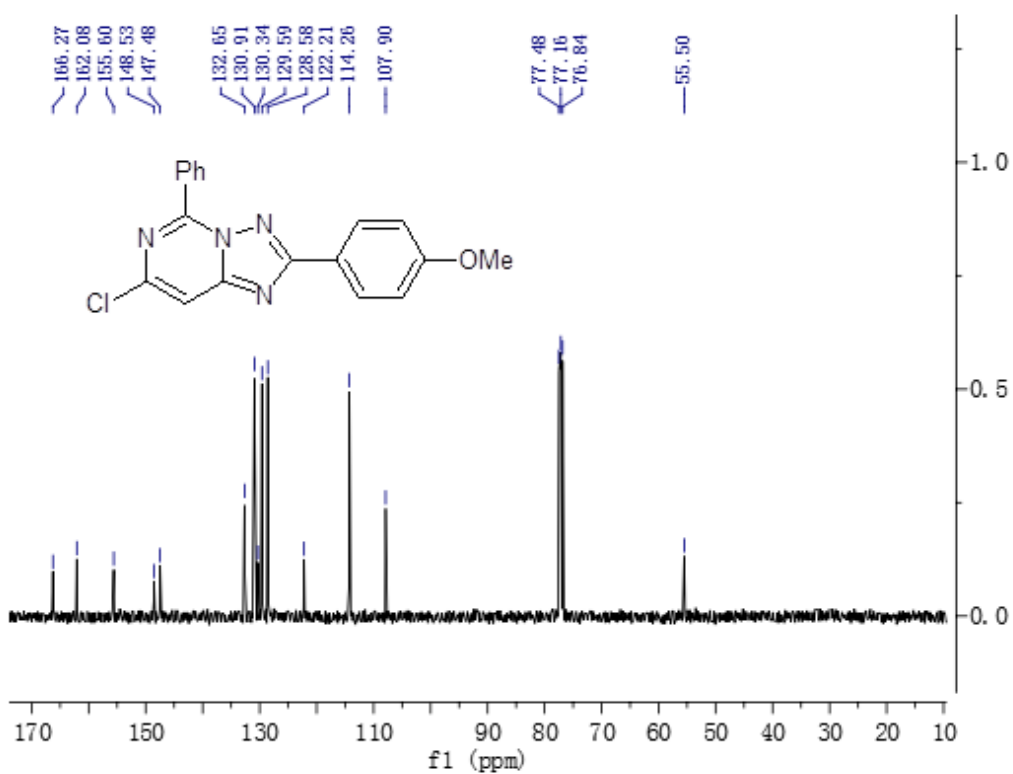
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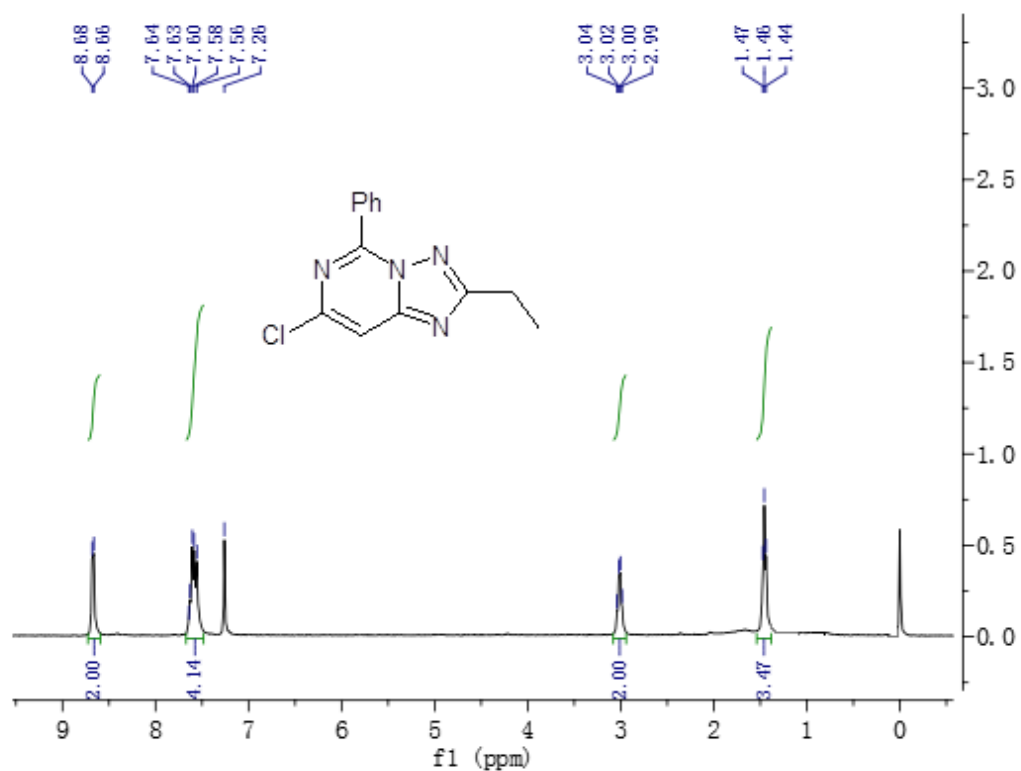
7-Chloro-2-(4-methoxyphenyl)-5-phenyl-[1,2,4]triazolo[1,5-c]pyrimidine (6n)



7-Chloro-2-(4-methoxyphenyl)-5-phenyl-[1,2,4]triazolo[1,5-c]pyrimidine (6n)



7-Chloro-2-ethyl-5-phenyl-[1,2,4]triazolo[1,5-c]pyrimidine (6o)



7-Chloro-2-ethyl-5-phenyl-[1,2,4]triazolo[1,5-c]pyrimidine (6o)

