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A Carbodiimide-Mediated Synthesis of Pyrimidothienopyridazine Derivatives *via* a Tandem Nucleophilic Addition-Intramolecular Hetero Conjugate Addition Annulation Strategy

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Introduction

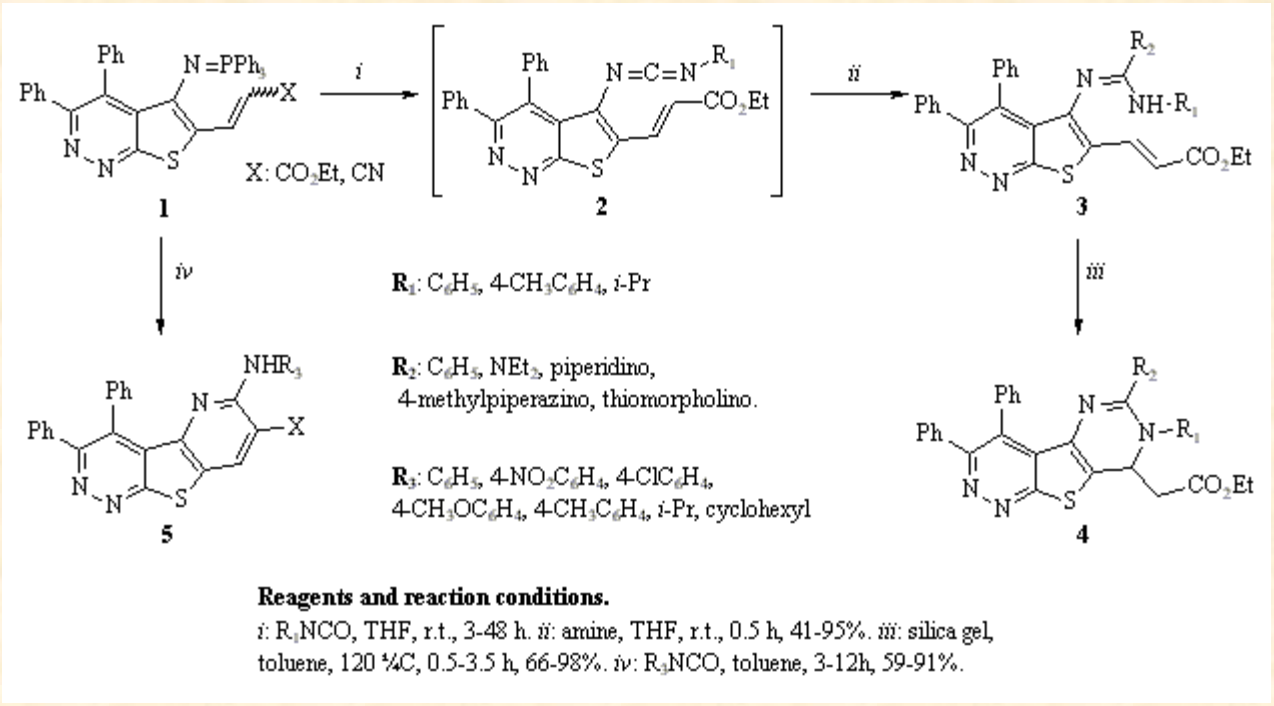
Over the past decade, great progress has been made in the field of heterocyclic synthesis by the aza-Wittig methodology. The key intermediate iminophosphoranes can be prepared either by the Staudinger reaction from organic azides or by Kirsanov reaction from primary amines.

Previously, we described an efficient synthesis for pyrimidothienopyridazines derivatives *via* intramolecular aza-Wittig reaction heterocyclization strategy.[1]

In this communication, we report the synthesis for pyridothienopyridazine and pyrimidothienopyridazine derivatives *via* aza-Wittig/electrocyclization and aza-Wittig/nucleophilic intramolecular hetero conjugate addition, respectively.

Results and Discussion

Iminophosphorane **(1)** derived prom heterocyclic *o*-aminoaldehyde underwent a facile aza-Wittig-type reaction with isocyanates to provide the carbodiimides **(2)**. Subsequent treatment with primary amines generated the guanidino-substituted intermediate **(3)**, which underwent intramolecular conjugated addition to give the fused pyrimidine **(4)**.



On the other hand, heating iminophosphorane **(1)** in toluene at 120 ^{O}C with isocyanates gave pyridothienopyridazine derivatives **(5)**. The formation of **5** can be understood to occur by initial aza-Wittig reaction to give the corresponding heterocumulene as intermediate; these last undergoes thermally induced 6p-electrocyclization of 2-aza-1,2,5-hexatriene moiety followed by a [1,3] hydrogen shift.

References

1. J.M. Quintela, R. Alvarez-Sarandés, M.C. Veiga, C. Peinador *Heterocycles*, in press.

Comments

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