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Title:	Synthesis of C2-Formamide(thiophene)pyrazolyl-C4'-carbaldehyde and their Transformation to Schiff's Bases and Stereoselective trans- β -Lactams: Mechanistic and Theoretical Insights
Authors:	Mandal, Sanjay K. (/jspui/browse?type=author&value=Mandal%2C+Sanjay+K.)
Keywords:	Schiff's Bases Vilsmeier-Haack reaction
Issue Date:	2022
Publisher:	Chemistry Europe
Citation:	ChemistrySelect, 7(37), 2202172
Abstract:	Herein, we describe synthesis of functionalized thiophenyl acetyl-hydrazones using acetyl-thiophene derivative as precursor which further underwent Vilsmeier-Haack reaction in an unexpected manner, providing three-carbon atoms to the molecular framework. The mechanistic view explained formation of C2-formamide(thiophene)pyrazolyl-C4'-carbaldehyde by three consecutive actions in single-pot: 1) nucleophilic amino to C2-iminium ion generation, 2) cyclization to pyrazole ring and 3) nucleophilic attack by pyrazole to C4'-iminium ion which finally leads to dual formylation in the system. This product burst to primary amines to synthesize highly substituted C2-formamide(thiophene)pyrazolyl-C4'-Schiff's bases. Further, the reactivity of synthesized Schiff's bases underwent metal-free ring closure with diverse heteroatomic ketene sources which exposed the emergence of stereoselective trans- β -lactams. The broad functional groups encircled monocyclic β -lactams were achieved in moderate to excellent yields under gentle conditions. Additionally, theoretical calculations on B3LYP/6-31G(d,p) level of some representative compounds are also investigated to support mechanistic explanation with their stabilized structures and physical properties.
Description:	Only IISERM authors are available in the record
URI:	https://doi.org/10.1002/slct.202202172 (https://doi.org/10.1002/slct.202202172) http://hdl.handle.net/123456789/4466 (http://hdl.handle.net/123456789/4466)
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