Title:	Stereoselective synthesis and characterization of novel trans-4-(thiophenyl)pyrazolyl-β-lactams and their C–3 functionalization
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Abstract:	A stereoselective synthesis and C–3 functionalization of a long series of novel hybrid 4-(thiophenyl)pyrazolyl-β-lactams have been carried out. The divergent substrate scope and mechanistic insights were examined to delineate the generality of reaction that favored trans-β-lactams 4a-q almost exclusively in all cases. The C–3 functionalization was achieved by Lewis acid assisted nucleophilic substitution reaction of cis-3-chloro-β-lactams 6a-e to afford cis-3-monosubstituted-β-lactams 7a-e. The cis stereochemistry of β-lactams 7a-e was further established by stereospecific desulfurization with Raney-nickel, in representative cases (7a,b), leading to the formation of cis-β-lactams 8a,b. The structures and stereochemical assignments for synthesized β-lactams have been unambiguously confirmed using FT-IR, 1D NMR (1H and 13C), 2D NMR (1H–1H COSY, 1H–13C HSQC and 13C DEPT–135), elemental analysis (CHN), mass spectrometry (ESI-MS) and single crystal X-ray crystallography, in representative cases (4b,e). The cis and trans configuration of the hydrogen/chloro/nucleophile substituent at C–3 was assigned with respect C4–H of the β-lactam ring.
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