Synthesis of 3-(Piperidin-4-yl)-6,7-dihydro-5*H*-pyrrolo-[2,1-*c*][1,2,4]triazole and Theoretical Study of the Hydrazone–Hydrazine Tautomerism of the Intermediate Hydrazonation Product

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Abstract—3-(Piperidin-4-yl)-6,7-dihydro-5*H*-pyrrolo[2,1-*c*][1,2,4]triazole was synthesized through a four-step process including etherification, hydrazonation, cyclization, and reduction with an overall yield of 39%. The final product was characterized by ^{1}H NMR and ESI–MS/MS. The molecular structures of benzyl (*Z*)-4-(2-(pyrrolidin-2-ylidene)hydrazine-1-carbonyl)piperidine-1-carboxylate and related compounds were analyzed using DFT calculations at the B3LYP/6-311+G(d,p) level of theory. The results indicated a higher stability of the hydrazone tautomers.

Keywords: 1,2,4-triazole; drug intermediate; tautomer; hydrazone–hydrazine tautomerism; density functional theory

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