Regioselective Synthesis, X-ray and DFT studies of new Indazolyl-thiazole derivatives

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Fused tricyclic systems containing pyrazole moiety have shown enhanced inhibitory activity against a variety of protein kinases and been found useful in the treatment of several cell proliferative disorders. We report herein the regioselective synthesis and biological activities of some new derivatives in continuation to our work on synthesis\(^1\)\(^-\)\(^3\) of antimicrobial agents. 1-Arylidene-2-tetralone, obtained from reaction of 2-tetralone and aromatic aldehydes, on condensation with thiosemicarbazide in acidic and alkaline medium afforded tetrahydro-2H-benzo[e]indazole-2-carbothioamide as cis and trans diastereoisomers of 1-H and 9b-H respectively. The synthesis of a new series of indazolyl-thiazol-4(5H)-ones from cis isomer and α-halo acids is reported. A DFT study along with single crystal X-ray diffraction data of a representative compound is presented. The reaction of indazole-2-carbothioamides with methyl iodide, DMAD and acetic anhydride are described. Newly synthesised indazolyl-thiazol-4(5H)-ones were screened for their antibacterial and antifungal activities. Some of the newly synthesised derivatives have shown promising antibacterial and antifungal activities.

References