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Molecular hybridization of two pharmacophores for the synthesis of a small library of pyrazole-thiadiazole conjugates and characterization by nuclear magnetic resonance (NMR) and infrared (IR) spectroscopy

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An increase in the incidence of infection and mortality due to bacterial and fungal infections, and the development of resistant species is of growing concern and emphasises the need for the continuous design and development of improved antibacterial and antifungal agents. Heterocyclic compounds (pyrazoles and thiadiazoles) are pharmacophores currently used in pharmaceutical agents due to their diverse pharmacological and biological activities. These are suitable scaffolds to consider when synthesising new and enhanced drugs. Molecular hybridization (MH) is a technique whereby multiple pharmacophores of bioactive scaffolds are combined to generate a single molecule with improved affinity and activity in comparison to the parent molecules. MH was used to synthesis and characterize a small library of pyrazole-thiadiazole conjugates, by first synthesising intermediates such as; hydrozone derivatives and thiosemicarbazone derivatives via the Schiff base formation, 4-formylpyrazole derivatives via the Vilsmeier-Haack reaction and finally the pyrazole-thiadiazole conjugates via oxidative cyclisation. The yield range for hydrozone derivatives was 35.07-94.37%, 4-formylpyrazole derivatives was 20.06-95.68%, thiosemicarbazone derivatives was 53.81-89.67% and pyrazole-thiadiazole conjugates was 20.96-79.63%. Final yields obtained for the 2-fluoro and 2-hydroxy substituted products were better than the 4-fluoro and 4-hydroxy hydrozone derivatives and final pyrazole thiadiazole conjugate. Final compounds were characterized by spectroscopic methods such as ^{1}H, ^{13}C and 2D NMR and IR. MH was a successful approach for this synthesis, which resulted in moderate to good yields, in comparison to literature values. The biological activity of these compounds will be analyzed to investigate their effects towards various bacteria and fungi.