Study on interaction of novel heteroaryl chalcones with calf thymus DNA using molecular docking and spectroscopic techniques

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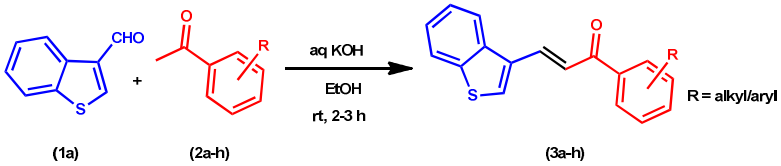
A series of new heteroaryl chalcone conjugates [Scheme 1, 3a-h] have been synthesized by Claisen–Schmidt condensation reactions of various substituted acetophenones (2a-h) with benzo[b]thiophene-3-carbaldehyde (1a). The heteroaryl chalcone conjugates thus obtained were characterized by IR, ^{1}H NMR, ^{1}H-^{1}H COSY, ^{13}C NMR, mass spectral analyses and single crystal XRD data and were found to be thermally stable up to 300 ºC. A large number of hybrid chalcones reportedly show anticancer activity [1,2]. In this study, automated docking was used to determine the orientation of the synthesised chalcones that bind to the CT-DNA [d(CGCGAATTCG CG)2 dodecamer (PDB ID: 1BNA)] obtained from the Protein Data Bank. Binding of these chalcones was studied using computational methods and biophysical studies. The results obtained from the binding study of the prepared compounds with CT-DNA at physiological pH will be presented along with molecular docking.



Scheme 1

References:

1. V Markovi, et al, *Eur J Med.Chem*; 89 (2015) 401.

2. C H Tseng, et al, *Eur J Med Chem*; 59 (2013) 274.