Abstract

The thesis entitled "**Design and synthesis of quinazolinones and related heterocyclic compounds**" deals with the synthesis of selected *N*-heterocycles with detailed mechanistic investigation accompanied by finding some of their applications.

The synthesis of functionalized Quinazolin 4-ones involving aromatic and aliphatic dialdehyde with amide has been established via Intramolecular hydride transfer (HT) or redox-neutral method. We proposed the hydride transfer mechanism based on the product obtained in a deuterated solvent. The influence of steric, electronic effects and length of the dialdehyde towards the hydride transfer reaction, have been investigated. NMR and mass spectrometry are used to characterize the synthesized quinazolinones. The simple methods are suitable for the preparation of a diverse array of multivalent quinazolinones.

We have also described the synthesis of a Donor–π-Acceptor Dihydropyrimidinone (DHPM) fluorophore via functional group modification of Dihydropyrimidinone to probe double stranded calf-thymus DNA. The intermediates including the target compounds was characterized by NMR, mass, and XRD. In order to find the general affinity of our synthesized compound towards double stranded-DNA, we have studied the various photo-physical properties with one of our compound i.e; Uv-Visible, Fluoresence, FL-lifetime, CD, comparative study with known dye etc. A theoretical model has been constructed by using the AutoDoc-Vina package to visualize different types of non-bonded interaction of the DHPM with other heteroatomic units in the narrow and shallow cut of the minor groove of ds-DNA. After finding the promising results as a DNA binder using ct-DNA as model, we treated SiHa cell line with the designed fluorophore. We observed selective localisation in the nucleus of the cell.

Herein, we reported an effective one-pot protocol to synthesize quinazolinone fused *N*-heterocyclic alkaloids, structurally similar to the natural product Luotonin and Rutaecarpine by $Pd(OAc)_2$/AgOAc-promoted intramolecular dehydrogenative cross-coupling (CDC). The electronic effect of the substituents attached to the backbone of the starting material was thoroughly investigated. The outcome of the reaction is highly dependent on the substrate structure and pH of the medium. Based on the experimental observation, a probable mechanism has been proposed. To see the anticancer properties, we have studied concentration-dependent cell viability assay of one compound on SiHa cell, a human cervical cancer cell line and observed IC_{50} value was 23 μM which is a good sign of applicability.

MA Mondal
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DR MOHABUL ALAM MONDAL
Assistant Professor
Department of Chemistry
Jadavpur University
Kolkata-700032, India

Sudipta Mondal.
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