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Diversity oriented synthesis of indole-based polyheterocycles in a one pot format

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Abstract

Despite paradigm shift in drug discovery from natural products to synthetic molecules to biologics, heterocycles have always remained as a major source for drug discovery. Two of the primary requirements for drug discovery pharmacokinetic (Solubility, lipophilicity, pKa etc) and pharmacodynamic properties (ability to access and bind the target) of test compounds in a focused library (against receptors or enzymes) can be regulated by generating structurally diverse annulated/tethered polyheterocycles with differential physico-chemical properties. In this direction, one–pot synthetic strategies leading to structurally diverse skeletal arrays offer opportunities for generating these libraries and have remained a challenging task for organic chemists. Such a format demand recruitment of substrates with multiple bond forming sites (atoms) which in turn, can be differentially exploited in one-pot afford structurally distinct products.

In our laboratory we had been regioselectively manipulating nucleophilicities of the three N-1, C-2 and C-3 positions in the indole for the generation of structurally diverse annulated polyheterocycles. Indoles belongs to a class of privileged structures that are present in a variety of drugs (>400) used clinically. We have employed appropriately functionalized indole derivatives and treated them with alkyne based reactants in a one-pot format via different annulation pathways. In general, either a three component domino/tandem reaction or a two step protocol following MCR-post-MCR modification concepts has been applied for the construction of indole-based polyheterocycles. The current challenges in designing one-pot strategies for the diversity oriented synthesis of indole-based polyheterocycles by CH/NH activations will be also discussed.

Biography

Dr Bijoy kundu was Former Chief Scientist in Medicinal & Process Chemistry Division at Central Drug Research Institute- CSIR, India

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