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Synthesis of Bioactive Molecules using Green Chemistry Techniques

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Abstract: *Most of the bioactive molecules are synthesised by time-consuming conventional methods. The use of toxic chemicals harms the environment and human beings. In this review, an attempt has been made to introduce methods and procedures related to the green and environment benign synthetic process. Until 1980's the knowledge of the risks associated with using chemicals was quite poor among the chemists. This review mainly focuses on the green synthesis of Indazoles, Benzimidazoles, Coumarins, Pyrazoles and Imidazoles. As on today, toxicity of the chemicals can be explained to eliminate the cause of its toxicity without sacrificing the desirable properties of the chemical.*

Keywords: Indazoles, benzimidazoles, coumarins, imidazoles, green catalysis, solvent free reaction.

I. INTRODUCTION

Green chemistry is an eco-friendly and an efficient method for the synthesis of most of the chemical entities. It is helpful to reduce the carbon footprint in the field of synthetic chemistry. Green chemistry prevents the pollution at molecular level. Green chemistry uses efficient solvents and catalysts for the synthesis of drug molecules. This method reduces the environmental pollution and prevents the toxic effect of chemicals on human and animals. It involves different green methods useful in the field of the organic chemistry, medicinal chemistry and chemical engineering. Microwave irradiation and Sonochemistry are good source of heat as compared to the conventional heating techniques. The effect of microwave irradiation creates superheating effect directly inside the solvent. Sonochemical reactions produce adiabatic process without affecting the molecule. These techniques are helpful in the minimisation of waste products and time required for the chemical reaction2, 3 . These techniques reported with high yield and quality product in the synthesis of quaternary ammonium salts, quinalinimides, and hydantoins4-6 . Solvents play a vital role in synthetic reactions as reaction media. In this category, green solvents are best as compare to petrochemical solvents. Green solvents like supercritical carbon dioxide, aqueous hydrogen peroxide play a vital role in green chemistry. These solvents are less toxic, biodegradable and derived from renewable sources 8, 9 . The use of solvents in the organic synthesis is a common practice from decades. However, chemists concern to reduce the environmental pollution caused by solvents. These reactions achieved by use of the biocatalysts embedded in the clays, zeolytes, silica, alumina or other matrices with the thermal effect of UV, microwave irradiation or ultrasound effect. 10 Most of the synthetic reactions do not take place without catalyst. Green catalysis11 is sustainable method to increase the rate of reaction with fewer intermediates. The use of Biocatalysts, Clays, Noble and non-noble metal complexes leads a sustainable green syntheisis. Green synthesis without protecting groups is more convenient to reduce the unnecessary generation of intermediates. A protection/deprotection lengthens the reaction steps, incurring the cost for additional reagents and waste disposal, and finally leads to a reduced overall yield. Here we present relevant historical context and highlight recent total syntheses that have developed new chemistry in an effort to exclude protecting groups.12 Overall, this

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review explores the different green and efficient techniques used for the synthesis of the various potent biologically active molecules like Indazoles, Benzimidazoles, Coumarins, Pyrazoles and Imidazole.

The creation of substitute techniques for the bioactive heterocyclic precursor's production is the focus of green chemistry4 . Fig.1 illustrates these processes, which involve lowering the usage and manufacture of hazardous materials as well as the creation of byproducts in the form of nonrenewable materials. The foundational concepts encapsulated in the "twelve principles of green chemistry" serve as the bedrock of inquiry within this discipline. These 12 rules help set goals for developing more resilient and environmentally friendly chemical processes5 . While optimising all 12 criteria would be ideal, in practise it might only be possible to optimise a few.

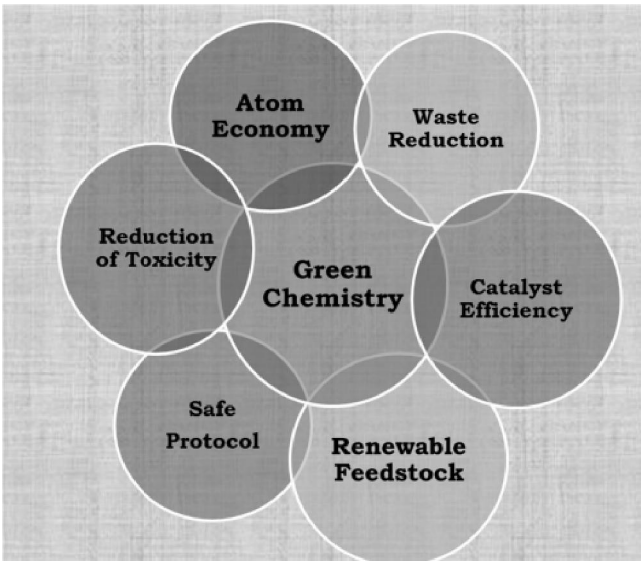

Fig. 1 Summary of Principles of Green Chemistry

II. GREEN TOOLS IN SYNTHESIS OF BIOACTIVE HETEROCYCLIC

An overburden in the chemist and scientist community has emerged due to the environmental safety issue. Nearly 40% of environmental pollution is due to chemicals that are hazardous to the ecosystem. To avoid the problem of pollution, the following green tools for organic synthesis can be used:

A. Iconic Liquids in the Synthesis

Ionic liquids, called ILs, are naturally occurring molten salts. The research community has shown a considerable deal of interest in ionic liquids (ILs). Due to their remarkable attributes, including non-flammability, low vapor pressure at ambient conditions, solvent capabilities, superior thermal and electrochemical stability, recyclability, high polarity, and low viscosity at room temperature, ionic liquids are utilized as catalysts in various reactions.

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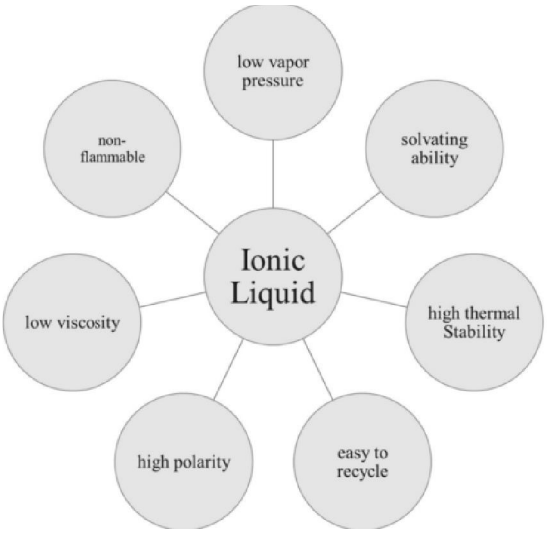

Fig 2: Chiastic feature of ionic liquid for synthesis of various scaffolds

Scheme 1 illustrates a sustainable and efficient approach for synthesizing aminoalkyl naphthol derivatives through multicomponent reaction involving substituted aldehydes 2- naphthol with amide derivatives, employing the catalyst 5-mol% of 2-methyl pyridinium trifluoromethane sulfonate ([2-MPyH]OTf)7 . An effective technique has been devised for the one-step synthesis of amidoalkyl naphthols employing diverse solvents as eco-friendly and sustainable catalysts. This method yields a broad spectrum of biologically active heterocyclic intermediates, as depicted in scheme 28 . Yinglei Wang and colleagues have introduced an innovative approach for the single step synthesis of dihydropyrano[3,2-c]chromene, demonstrated in scheme 3. This method employs unique poly(ethylene glycol)-linked N,Ndimethylamino pyridine modified dicationic ionic liquids and facilitates a multicomponent reaction condensation involving aryl aldehydes, malononitrile and 4-hydroxy-2H-chromen-2-one in an aqueous environment9 . Scheme 4 outlines the novel method devised by Patel et al. for the one-step synthesis of bis(indolyl)methane compounds utilizing [DSIM] [AlCl3]x-@CS chitosan-aided ionic liquid (CSIL). This process involved the utilization of various modified benzaldehydes10. Using [EMIM]AlCl4 substrate for the production of 3,4-dihydropyrimidin-2(1H)- one and thione derivatives, Popatkar et al. devised a novel Biginelli production technique, as illustrated in scheme 511. M. Shaheer Malik et al. proposed a new strategy for cyclocondensation of four components to synthesize novel indole-pyran hybrids (scheme 6) based on phthalazinones employing ionic liquids. Also, a few derivatives that were synthesized had considerable activity, exhibiting IC50 values ranging from 5.8 to 9.6 lM. According to in silico docking studies, derivatives were identified to possess significant binding affinity, measured at 11.2 and 10.2 kcal/mole, respectively, towards the human tankyrase-1 enzyme12. Yuan Yu and colleagues introduced an innovative approach for the enzymatic synthesis of 4H-pyrimido [2,1-b] benzothiazole scaffolds, as depicted in scheme 7. They further investigated the potential of these scaffolds for lysosome targeting through a multi component Biginelli reaction involving aldehyde, β-ketoester, and 2-amino benzothiazole. A small number of synthesised motifs have the AIE (Aggregation-Induced Emission) feature, which may be a biomarker13.

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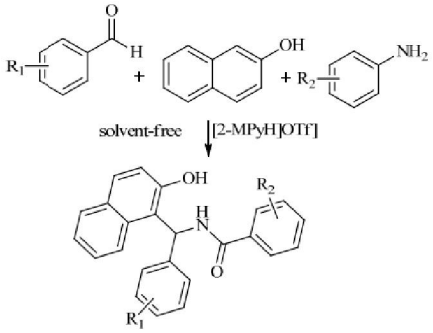

Fig 2: Scheme 1

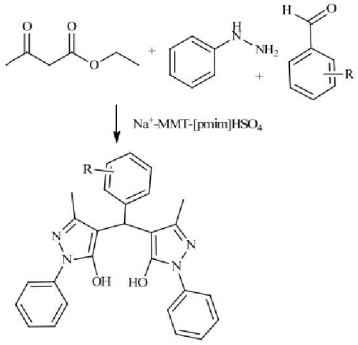

Fig 3: Scheme 2

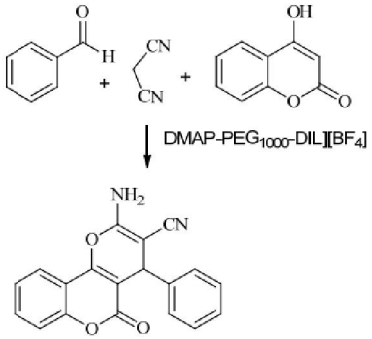

Fig 4: Scheme 3

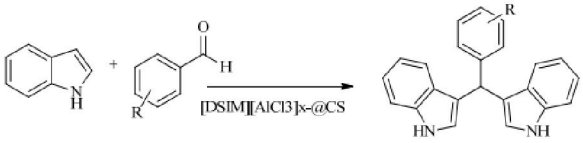

Fig 5: Scheme 4

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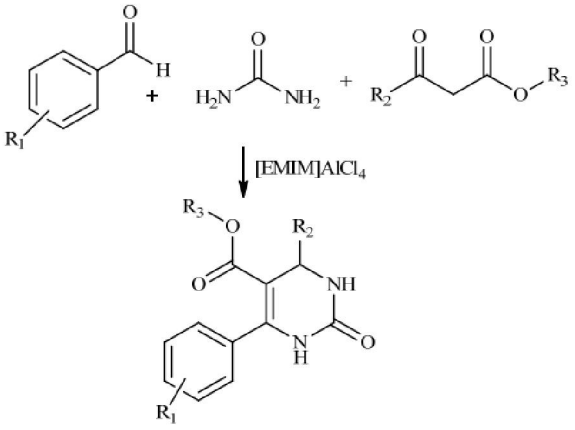

Fig 6: Scheme 5

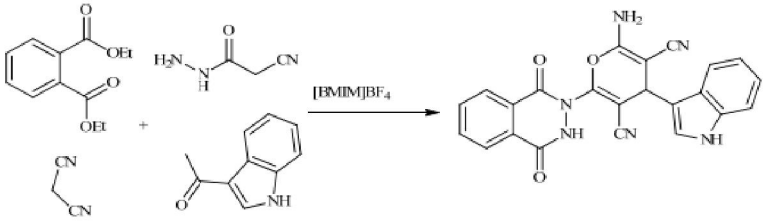

Fig 7: Scheme 6

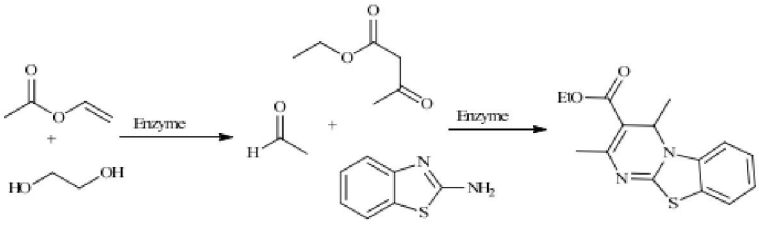

Fig 8: Scheme 7

III. ARTIFICIAL INTELLIGENCE IN GREEN CHEMISTRY

The development of technological advances is intended to free people from laborious work, improve their capacity for nature observation, and increase their accessibility to communication. It has long been held that only people are capable of learning, offering solutions, and reaching judgments62. Artificial intelligence has seen a huge increase in chemical applications in recent decades. Artificial intelligence represents one of the subjects in chemistry that is discussed the most. Chemistry and artificial intelligence go hand in hand. Chemistry along with artificial intelligence are primarily employed in the healthcare industry to produce new medications. The combination of medical science and technology has resulted in significant changes to the manufacturing and preparation of pharmaceuticals63. Indeed, with the rapid advancements in computer science and engineering in recent years, artificial intelligence has expanded its range of applications significantly64. Scientists create reaction arrays to optimise the efficiency of couplings amongst building components. Pharmaceutical study frequently uses the Suzuki coupling, Buchwald-Hartwig coupling, and amide coupling. Based on the collection of literature, the established artificial intelligence model of language ChatGPT may generate reply arrays for these typical responses65. In Figure 3 we glimpse on range of artificial intelligence in

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chemistry and related domains including material science includes designing new compositions of materials for specific applications, controlling air and water pollution by designing green chemistry-based AI techniques, predicting retro-synthetic routes for natural products synthesis, drug discovery using software like docking studies, predict route drug delivery in clinical application, simply the different aspect of chemistry by educational videos, and useful to designing new material66.

IV. CASE STUDY

Heterocyclic compounds are essential in drug discovery due to their diverse biological activities. This case study highlights green techniques for synthesizing bioactive heterocycles, emphasizing sustainability and reduced environmental impact. Green synthesis methods such as microwaveassisted, ultrasound-assisted, and flow chemistry have gained prominence for their efficiency in generating heterocyclic compounds. These techniques reduce reaction times, solvent usage, and waste generation. Microwaveassisted synthesis, for instance, allows for precise temperature control and significantly shorter reaction times, minimizing energy consumption. Utilising bio-based raw materials and renewable feedstocks in order to lessen dependency on resources that are not renewable is another ecological strategy. Moreover, catalysis plays a crucial role in green heterocycle synthesis, enabling milder reaction conditions and reduced by-product formation. Case in point, the synthesis of bioactive quinoline derivatives using microwave-assisted catalysis with recyclable catalysts and benign solvents. This approach not only expedites the process but also decreases the environmental footprint. In summary, green techniques for heterocycle synthesis promote sustainability by reducing waste, energy consumption, and reliance on non-renewable resources, making them a crucial aspect of modern drug discovery and chemical research. These practices align with the growing emphasis on environmentally friendly processes in the pharmaceutical industry.

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