

Significance of Heterocyclic Compounds in New Drug Development

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Heterocyclic Compounds possess a non-carbon atom other than carbon in their ring Structure. The presence of atoms like Nitrogen, oxygen, and sulfur, which provide Versatility, electron Multitarget interactions, Pi-Pi Stacking, and donor-acceptor features to these Compounds. The formation of Wander-Walls, hydrophobic and metal-coordination bonds make these compounds versatile, with a wide range of ring sizes, shapes, and structural permutations. They play a role in Metabolism and biochemical processes. A stable binding with a receptor is essential for a drug's biological activity. A covalent bond formed is an irreversible activity, and non-covalent bonds provide a reversible action. Drugs that contain a heterocyclic ring can be anticancer, anti-inflammatory, neuroprotective, or antiviral. They possess structural diversity, optimal physicochemical properties, and the potential for lead optimization. Thiazoles, triazoles, Pyridine, furans, and quinolines form part of many drugs. Phytochemical with a heterocyclic nucleus, like quinines. Synthetic dyes like isoniazid and Fluoxetine contain Nitrogen in their rings. They are part of DNA, proteins, and vitamins; rings are 5 or 6-membered, saturated or unsaturated.

The Lipinski rule of 5 and the fragment rule of '3' are used to guide lead optimization of heterocyclic ring compounds. The diversity and versatility of heterocyclic compounds make them good drug candidates. Triazoles, Benzimidazoles, Pyrazolines, Pyrans, Tetrahydrofuran, and furans are recently utilized for drug discovery. The fluorine atom (F) in the ring system of a compound enhances the biological activity. The Phyto-Compounds flavonoids. terpenoids, alkaloids possess, anti-cancer, anti-oxidant, anti-inflammatory and anti-microbial, anti-malarial activities. Phytochemicals are less toxic, readily available, multitarget binding and possess natural healing properties. The use of artificial intelligence in Computational Chemistry and drug discovery has had a positive impact, boosting and simplifying the process.