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An Exploration of the Medicinal Chemistry of Anticancer Quinoxaline

Luis Polo Parada*

Assistant Professor,Department of Medical Pharmacology and Physiology,University of Missouri,USA

Introduction

Quinoxalines are benzopyrazines with fused benzene and pyrazine rings. Due to their distinct pharmacological activities, quinoxalines have recently piqued the interest of Medicinal Chemists for their syntheses and chemistry. Various synthetic protocols, such as multicomponent reactions, single pot synthesis and combinatorial approaches using efficient catalysts, reagents and nano-composites, have been developed. Furthermore, the quinoxaline core's versatility and reasonable chemical simplicity make it an extremely promising source of bioactive compounds. As a result, many bioactive quinoxalines have been developed as antitumor, antifungal, anti-inflammatory, antimicrobial and antiviral agents [1].

Description

One of the most important and well-studied branches of medicinal chemistry is heterocyclic organic chemistry. The various constituent heteroatoms of heterocyclic bioactive compounds, such as nitrogen,1,2 sulphur,3-6 oxygen,7,8 and others, are an important feature. 9 These heteroatoms have a direct impact on the reactivity of the target skeleton, the activity (or toxicology) of the compounds, interactions between target drugs and different target inhibitors and can influence metabolism and pharmacokinetics [2].

Natural, synthetic and hybrid compounds that are biologically relevant are a great resource for lead formation and the development of novel pharmaceuticals. Wu et al.52 recently synthesised 60 novel 1,2,3-triazole-containing pharmacophores related to allogibberic acid fragments. The cytotoxic potential of all hybrid allogibberic triazole hybrids was determined using the A-549, HL-60, SMMC-7721, MCF-7 and SW480 cell lines. The most potent compound demonstrated significantly greater cytotoxicity than the positive control drug cisplatin against all five tumour cell lines tested, with IC50 values ranging from 0.25 to 1.70 M [3].

The substitution of an amide group for a heterocyclic ring in a bioactive molecule can have a significant impact on its physicochemical and pharmacological properties. This substitution adds structural rigidity to the compound, which may result in compounds with improved potency, selectivity, metabolic stability and PK properties. Triazoles, imidazoles, oxadiazoles, oxazoles, isoxazoles, imidazolidinones, triazolones and many six-membered heterocycles that retain the geometry of the amide bond or maintain the hydrogen bond (H-bond) accepting/donating properties of the amide group yield many successful examples.

The discovery of the HIV-1 integrase inhibitor raltegravir demonstrated the role of 1,3,4-oxadiazole as an effective amide isostere in modulating potency shift in cell-based antiviral assays using 10% heat-inactivated foetal bovine serum (FBS) or 50% normal human serum. In contrast, the thiophene analogue, which was predicted to have a nonplanar preferred conformation, was about 10-fold less potent than the progenitors, supporting the hypothesis that the planarity of the amide linker was required for potency. Further refinement of the oxadiazole and oxazole analogues by the addition of extended amine groups on the oxadiazole and oxazole rings identified a clinical candidate for the treatment of respiratory indications via inhalation [4,5].

Conclusion

The preceding discussion and observations demonstrated that this promising moiety has a lot of potential. Future efforts could include the development of novel catalytic systems to broaden the substrate range of quinolones. Over the last decade, significant progress has been made in the design and development of quinolone-based anticancer and antiprotozoal agents with high pharmacological activity and improved physicochemical properties. Quinolones and their derivatives are thus promising scaffolds for cancer and malaria chemoprophylaxis and treatment. Furthermore, some of them have already been used in clinics or are in various stages of clinical development for the treatment of the aforementioned diseasesQuinolone motifs' extensive biological profile and pharmaceutical properties, as well as their structure-activity relationship properties, will undoubtedly lead to the development of potential pharmaceutical agents. We hope that this literature inspires more exciting research in various disciplinary fields and provides useful information about how a medicinal chemist can use the quinolone nucleus to design and develop clinically viable molecules for the treatment of various devastating diseases.

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***Address for Correspondence:** Luis Polo Parada, Department of Medical Pharmacology and Physiology,University of Missouri, USA, E-mail: luispoloparada@gmail.com*

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Conflict of Interest

There are no conflicts of interest by author.

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