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RESEARCH ARTICLE

In Silico Exploration and Synthesis of New Quinazolinones as Antimicrobials using a Computational Approach

Amit Kumar[1,*] and Sushil Kumar[1]

[1]*School of Pharmaceutical Sciences, Faculty of Pharmacy, IFTM University, Moradabad (Uttar Pradesh), India*

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Abstract: ***Introduction*:** The microbial infections are amongest the most common health problems and now a days existing drugs showing ressistant against microbial infections. Therefor, new quinazolinones have been explored.

***Materials and Methods*:** The target compounds were formed using a synthetic method and confirmed by spectral analysis. The synthetic achievement, Benzoxazinone (3), was derived from anthranilic acid (1) and aromatic acid chloride (2) in the presence of pyridine, and further reacted to aminoacetophenone (4) formed 2-phenyl-amino-quinazolinone (5), afforded to then intermediate derivatives (7) react with *p*-chlorobenzaldehyde (6), then further reacted with substituted amines, with copper iodide, and refluxed, 15 h, in a flask containing anhydrous dimethylformamide, potassium carbonate to formed the targeted newer quinazolinone derivatives (A8a-j) shown in the Scheme **1**.

***Results*:** In the results, we showed that the newer quinazolinone compounds A8b and A8f have been the two best compounds out of ten. The molecules were showed good computational parameter, including molecular dynamics simulations, docking scores, and physicochemical properties, when compared to the reference drugs. To examine the computational and structural basis of the relation between the test for *in vitro* antimicrobial activity.

***Discussion*:** The computational properties were performed for the designed molecules. Compounds, A8b and A8f were showed good *in silico* studies against *S. aureus*, *E. coli* and *A. niger*, and further synthesized and characterized by spectrals and analytical methods.

***Conclusion*:** In conclusion, compounds (A8b & A8f) showed good antimicrobial properties, which supported by *in silico* studies. The findings confirm that newer quinazolinone derivatives have the most promising relationships between *in silico* studies and biological validation for the next generation of antimicrobial agents.

Keywords: Quinazolinones, amines, ADMET studies, molecular docking, MD simulations, antimicrobial activity.

1. INTRODUCTION

Quinazolinones are privileged in the framework of medicinal chemistry for the discovery of novel bioactive pharmaceuticals and diverse biological activities [1, 2]. Quinazolinones are a class of heterocyclic chemical compounds characterized by a benzene nucleus fused to a pyrimidine, featuring a keto or oxo group at the 4-position, referred to as quinazolin-4(3*H*)-one. The strong aromaticity of the ring and the presence of heteroatoms have been linked to the quinazolinone molecules' diverse *in vitro* antimicrobial activity, as illustrated in Figs. (**1a-d**) [3, 4]. Quinazolinones have the most effective medicinal properties, including antibacterial, antifungal, and anticancer properties, *etc* [5-7].

In terms of chemistry, quinazoline and quinazolinone together form a significant class of six-membered fused heterocyclic or aromatic rings [8-12]. This involves incorporating two conjoined aromatic rings with two nitrogen atoms and the oxidation of one carbon with a keto oxygen [13-15]. The computational studies were employed in various distinct methods to establish the correlation between the different calculated studies of the designed molecules [16, 17]. In the recent study, a series of derivatives based on the quinazolinone motif were *in silico* designed, synthesized, and characterized for evaluation against the antibacterial and antifungal targets [18-26]. In view of the continuing need to develop potential and selective antimicrobial agents, we have designed, synthesized, characterized, and evaluated the

*Address correspondence to this author at the School of Pharmaceutical Sciences, Faculty of Pharmacy, IFTM University, Moradabad (Uttar Pradesh), India; E-mail: amitkumarbph@gmail.com

