

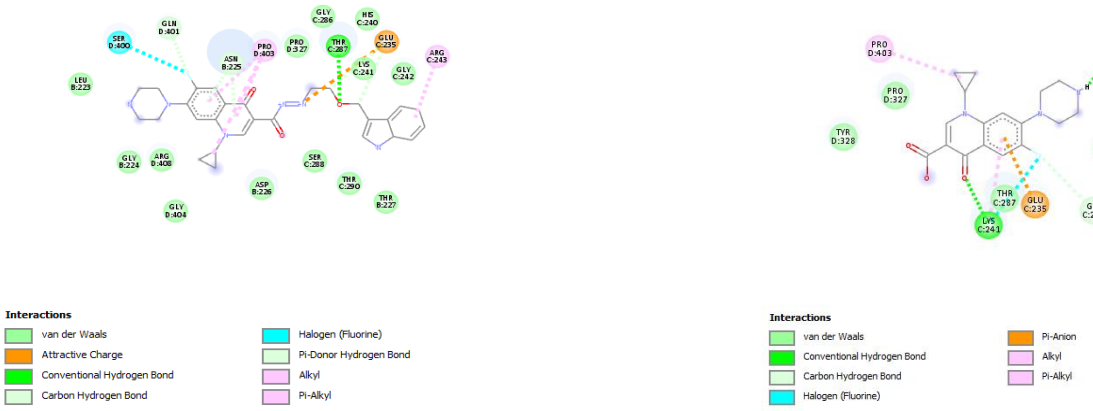
DESIGN AND COMPARATIVE *IN SILICO* ACTIVITY OF CIPROFLOXACIN/CAFFEIC ACID CONJUGATES AS COMBINED GYRASE AND PRIMASE INHIBITORS

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According to WHO, the global burden of microbial infections causes about 700,000 deaths each year. This is accompanied by an increasing rate of antimicrobial resistance (Kim and Hooper, 2014). Therefore, the need for new antimicrobial molecules cannot be overemphasized. Preliminary *in silico* docking studies (using PyRx Software) of eight (8) designed conjugates showed better docking scores (binding affinity) on both gyrase and primase enzymes compared to the parent molecules (ciprofloxacin and caffeic acid). More so, both PASS Software and ProTox Software showed appreciable *in silico* antimicrobial activity and limited organ toxicity respectively compared to the parent molecules. Consequently, this project seeks to fully design these molecules as lead-conjugates possessing both gyrase and primase inhibitory activities. The lead-conjugates will subsequently get synthesized, fully characterized and subjected to antimicrobial evaluation.



1 2

Figure 1: Ciprofloxacin conjugate (1) showing better interaction compared to ciprofloxacin molecule (2).

Biography

Naruka Solomon Yakubu is currently a PhD Student in the Department of Pharmaceutical and Medicinal Chemistry, Faculty of Pharmaceutical Sciences, University of Jos, Nigeria under the supervision of Prof. E.O. Afolabi. Mr Naruka has completed his Masters' degree in Pharmaceutical

Chemistry in 2017 and a Bachelor degree (B.Pharm.) in 2007 from the University of Jos. He is currently a Lecturer II in the Department of Pharmaceutical and Medicinal Chemistry. He has published about 5 papers in reputed journals. He is a passionate researcher with core interest in Synthesis, Drug Discovery and Development and Computational Chemistry.

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