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Design and virtual screening of potential CD14inhibitors with focus and chlorogenic acid as Lead

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Abstract

 $\mathbf{P}_{\text{harmacovigilance (PV)}}$ is defined according to WHO, as the science and activities relating to the detection, assessment, understanding and prevention of adverse effects or any other drug-related problem. The aims of PV are to enhance patient care and safety in relation to the use of medicines; and to support public health programmes by providing reliable, balanced information for the effective assessment of the riskbenefit profile of medicines. In silico methods are primarily used alongside the generation of *in vitro* data both to create the model and to test it. Such models have seen frequent use in the discovery and optimization of novel molecules with affinity to a target, the clarification of absorption, distribution, metabolism, excretion and toxicity properties as well as physicochemical characterization. Cheminformatics plays a key role to maintain and access enormous amount of chemical data, produced by chemist by using a proper database.



Biography:

Olanike Catherine Poyi currently works at the Department of Pharmaceutical and medicinal chemistry, University of Jos, Plateau Stat, Nigeria. Olanike does research in Drug Design, Bioinformatics, Medicinal, Computational and synthethic chemistry. She has published several papers in reputed journals.

Speaker Publications:

1. "Design, Molecular Docking And In Silico Analysis Of Analogues Of Chloroquine And Hydroxychloroquine Against SARs-COV-2 Target (6w63.pdb)"

2. "Phytochemical Compounds Present in COVI-MXG Herbal Preparation Inhibits RNA-Dependent RNA Polymerase from SARS-CoV-2: Virtual Screening"

3. "In-vivo Studies of the Effect of a Herbal Preparation on Pharmacokinetic Properties of Rifampicin in Male Swiss Albino Rats and Computer Mediated Mechanism of Interaction"

4. "in-vitro and in-silico drug-food interaction: an evaluation of Metformin and green tea interactions"

5. "Design and docking studies of inhibitors for the chorismate synthase from Streptococcus pneumoniae using 5-enol pyruvylshikimate 3-phosphate (EPSP) analogues"

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