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RESEARCH ARTICLE

# Assessing the Antimalarial Potentials of Phytochemicals: Virtual Screening, Molecular Dynamics and *In-Vitro* Investigations

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**Abstract:** ***Background*:** Combined *in-silico* and *in-vitro* approaches were adopted to investigate the antiplasmodial activity of Catharanthus roseus and Tylophora indica plant extracts as well as their isolated components (vinblastine, vincristine and tylophorine).

***Methods*:** We employed molecular docking to prioritize phytochemicals from a library of 26 compounds against Plasmodium falciparum multidrug-resistance protein 1 (PfMDR1).

***Results*:** The retrieved bioactive compounds viz. tylophorine, vinblastin and vincristine were found to exhibit significant interacting behaviour; as validated by *in-vitro* studies on chloroquine sensitive (3D7) as well as chloroquine resistant (RKL9) strain. Furthermore, molecular dynamics (MD) simulations were performed for a duration of 10 ns to estimate the dynamical structural integrity of ligand-receptor complexes.

***Conclusion*:** We anticipate that the retrieved phytochemicals can serve as the potential hits and presented findings would be helpful for the designing of malarial therapeutics.

**Keywords:** Malaria, *Pf*MDR1, docking, schizont maturation assay, *plasmodium,* molecular dynamics.

## 1. INTRODUCTION

Malaria is among the "big three" infectious diseases and one of the prime causes of mortality and morbidity in tropical and subtropical regions of the world [1-3]. As per census records, 296 million (148-304 million) new cases of malaria worldwide were reported that account for 7,31,000 deaths [4-6]. It is further estimated that, in every 40 seconds, a child dies due to malaria resulting in a daily loss of more than 2000 young lives worldwide [7]. Owing to widespread researches, these numbers are decreasing but still remain epidemic and prevalent [8].

Current drug discovery related approaches use the multi-faceted ways to combine botanical, phytochemical, biological, and molecular modeling techniques [9-11]. In this course, medicinal plant drug discovery provides new and diverse functionalities for developing novel *lead* molecules against various pharmacological targets [12]. Besides, the phytochemical derived information and traditional medicine (ethnomedicine) are pertinent for corroborating new drug discovery campaign [12]. Recently, various drug screening approaches are being developed to improve the ease of data mining and virtual screening techniques against the library of phytochemicals [13-15]. It is hoped that more efficient and effective application of phytochemicals will improve malaria-related drug discovery process [16].

In quest of probing ailment against malaria, plant-derived compounds have played an immense role in the development of several clinically useful agents. Perusing it, we have selected medicinal plants *Catharanthus roseus* and *Tylophora indica* (hereafter referred as *C. roseus* and *T. indica*) based on the ethnobotanical surveys that earlier had proved their adequacy in preventing infectious diseases [3]. To be more

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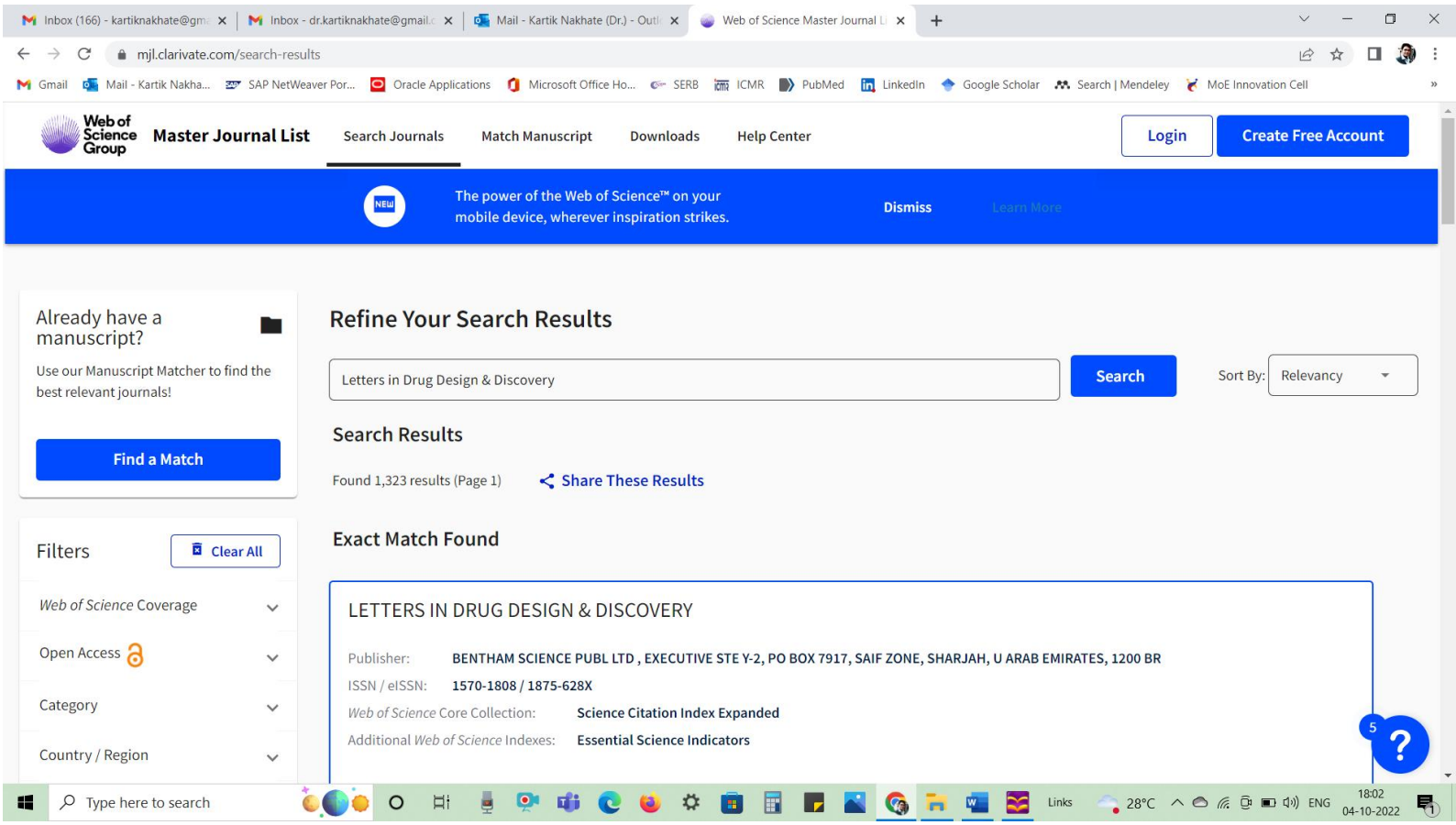
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