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Genes adaptability and NOL6 protein inhibition studies of fabricated flavan-3-ols lead skeleton intended to treat breast carcinoma

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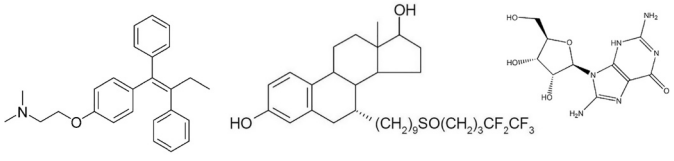
ABSTRACT

Breast cancer invasive 2.3 million women worldly and second prominent factor of cancer-related mortality. Finding a new site-specific and safe small molecule is a current need in this field. With the aid of deep learning Algorithms, we analyzed the published big database from cancer CBioportal to find the best target protein. Further, Multi-omics analysis such as enrichment analysis, scores of molecular, RNA biological function at a cellular level, and protein domain were obtained and matched to find the better hit molecules. The gene analysis output shows nucleolar protein 6 plays a significant responsibility in breast carcinoma and 354 natural and synthetic lead molecules are docked inside the active site. Docking result gave the output hit molecule falavan-3-ols with a binding score of −5.325 (Kcal/mol) and interaction analysis illustrates, 13 active amino acids favoring the binding interaction with functional groups of the hit molecule compared to the standard molecule Abemacilib (−2.857 (Kcal/mol)). Best docked complex of flavan-3-ols and NOL6 protein subjected to dynamic simulation 100 ns to study the stability. The results proved that π-π stacked, carbon-hydrogen and electrostatic interactions are stable throughout the 100 ns simulation. The overall results conclude the hit molecule flavan-3-ol will be a safe and potent lead molecule to generate and treat breast carcinoma patients.

1. Introduction

Breast cancer is the most common cancer in women with an estimated 2.3 million breast cancer cases diagnosed annually worldwide [1–3]. Breast cancer develops in the lining cells (epithelium) of the glandular tissue's ducts (85 %) or lobules (15 %). The malignant development is initially contained inside the duct or lobule ("in situ"), where it often exhibits no symptoms and has a low risk of spreading (metastasis). These in situ (stage 0) tumors may develop over time and infect the breast tissue surrounding them (invasive breast cancer), then disseminate to surrounding lymph nodes (regional metastasis), or to other bodily organs (distant metastasis)

The researcher Swen Hoelder et al. [4] completely reviewed and stated the opportunities of small molecules in cancer therapy and listed the successful small molecules in breast cancer treatment [4]. Some of the current drugs which are used to treat breast cancer were shown in the structures significant



Tamoxifen **Fulvestrant** **Trastuzumab**

advancements in the treatment of breast cancer use of chemotherapy in the adjuvant settings we have seen a paradigm shift over the past few decades, using molecules of cyclophosphamide, methotrexate, 5-fluorouracil, and Anthracycline-based molecules. Outcome and patient safety in the short term. The long-term use of adverse effects of those medications to understand the adverse spectrum of whole chemotherapy. During the 1980s, anthracycline-based regimens using doxorubicin or epirubicin have been used extensively in the prophylactic treatment of

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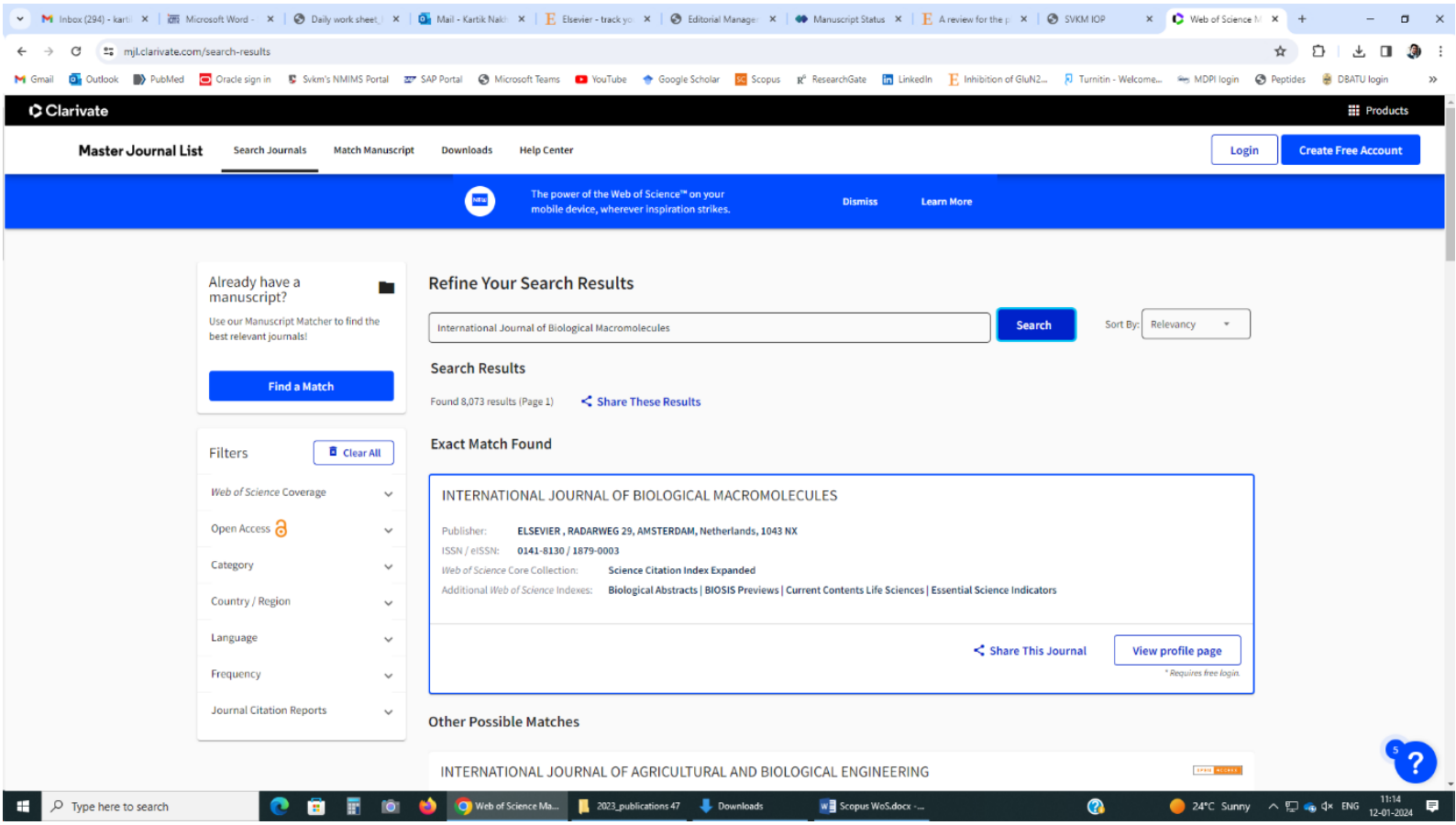
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