Available online at **www.joac.info**

ISSN: 2278-1862

Journal of Applicable Chemistry

2024, 13 (2): 98-113

(International Peer Reviewed Journal)

Evaluation of Some Designed Halogenated Variants of Gentisyl Alcohol: Molecular Docking, DFT, Druglikeness, and ADMET Studies for Assessing Biological Properties

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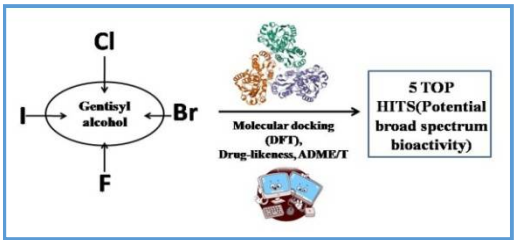
Accepted on 20th February, 2024

ABSTRACT

Antimicrobial resistance (AMR) poses a significant threat, complicating infection treatment and increasing the risks of severe illness. Concurrently, inflammation, prevalent in health issues like cardiovascular diseases, cancer, and diabetes, necessitates more effective therapeutic strategies. This dual challenge of AMR (Anti-microbial resistance) and inflammation underscores the critical need for novel and effective therapeutic. Incorporating halogen atom can profoundly alter a molecule's properties and may influence its bioactivity, metabolism, and pharmacokinetic profile. This study thus aims to design variants of gentisyl alcohol by incorporating bromine, fluorine, chlorine, and iodine atoms, evaluating their potential as antibacterial, anti-tubercular, antiviral, anti-parasitic, and anti-inflammatory agents via computational means. Employing molecular docking and Density Functional Theory (DFT), we assessed binding affinity, reactivity, and stability, alongside drug-likeness, pharmacokinetics, and toxicity. Compounds 7F, 4F, 7Br, 1F, and 7I exhibited superior and highest docking scores compared to gentisyl alcohol and native ligands against the target of interest with respect to PDB ID 7DQL, 3O4M, 4YRE, 7NNY, and 7OFS. Similarly DFT analysis revealed lower HOMO-LUMO energy gaps, suggesting enhanced and better stability and reactivity. These compounds met druglikeness criteria, demonstrated favorable ADME/T properties, and exhibited no signs of toxicity, indicating promise for drug development. Their high gastrointestinal absorption, moderate skin permeability, and absence of P-glycoprotein substrate activity further support their potential as lead compounds. In conclusion, compounds 7F, 4F, 7Br, 1F, and 7I shows potential in possessing broad-spectrum bioactivity and thus warrants further exploration and optimization for therapeutic applications.

Graphical Abstract:



Gentisyl Alcohol: Halogenated Variant's Molecular Docking, DFT, Druglikeness, and ADMET Assessment

Keywords: Molecular docking, DFT (density functional theory), ADME/T, Halogen.