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Antimycobacterial Effect of Naphthoquinone Natural Derivatives Identified in Henna leaves against Three Target Enzymes Computational Molecular Docking Study

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A B S T R A C T

Background:

Tuberculosis (TB) remains a major health threat, aggravated by rising drug resistance and treatment toxicity. Henna (*Lawsonia inermis*) is a plant commonly used in traditional medicine and folk cosmetics. The plant has topical anti-fungal effect, protect sunburn; topical analgesic and relief inflammation. However, their mechanism of action against *Mycobacterium tuberculosis* is not yet fully characterized.

Objective:

The present study aimed to evaluate the antimycobacterial effect of naphthoquinones natural derivatives from henna leaves extract against *M. tuberculosis* by computational approach targeting three essential *Mycobacterium* enzymes involved in bacterial growth and survival; and to identify the interactions between the derivatives and the target protein.

Methods:

The plant leaves were extracted by maceration in methanol and then subjected to GC-MS analysis and naphthoquinones derivatives were identified. Thereafter, the derivatives were investigated by molecular docking against mycobacterial target proteins including: Protein kinase G (PknG, PDB ID: 3CKQ), 4-diphosphocytidyl-2C-methyl-D-erythritol cytidyltransferase (IspD) and UDP-glucose-specific glycosyltransferase.

Results:

The docking results revealed that four Naphthoquinone compounds, 5-Hyroxy-1,4 Naphthoquinone, 2-Amino-3-chloro-1,4 Naphthoquinone and Coumarin-3-carboxylic acid exhibited binding affinities of −7.6, −8.2, −9.0, and −12.5 kcal mol^{-1} respectively, against protein kinase G, IspD and UDP-glucose-specific glycosyltransferase. Coumarin-3-carboxylic acid was a most promising candidate among the derivatives investigated achieved optimal binding stability and high inhibitory potential.

Conclusion:

The molecular docking analysis showed a significant antituberculosis potential of naphthoquinone derivatives found in henna leaves, particularly Coumarin-3-carboxylic acid as a promising lead for PknG inhibition. These findings provide a rationale for further biological validation and development of novel phytochemical-based therapeutics against drug-resistant TB. Further validating an *in vivo* activity of derivatives will be recommended.

Keywords: *Lawsonia inermis; GC-MS, Antimycobacterial, Naphthoquinone derivatives, Molecular Docking.*

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1. Introduction

Naphthoquinone derivatives found in *Lawsonia inermis* are recognized for their broad range of pharmacological properties, including potential applications in treating infectious and neoplastic diseases [1-2]. Naphthoquinones (NQs) represent a diverse class of phenolic compounds known for a spectrum of biological effects, such as antiviral, antibacterial, antiparasitic, anti-inflammatory, anticancer, and antifungal actions[3]. The antibacterial drug irrational use led to different microorganisms have emerged with enhanced resistance. Also, many of these drugs have shown potential adverse effects in humans. As global epidemic, *Mycobacterium tuberculosis* strains are emerged multi-drug-resistant threatening progress. *M. tuberculosis* is intrinsically resistant to many antibiotics, limiting the availability of effective treatment. Therefore, it has been a mounting in the efforts to discover or develop novel antimicrobial agents[4,5]. NQs unique chemical structure allows them to interact with biological molecules, and modifications can lead to more effective therapeutic agents. The continuing exploration of naphthoquinone derivatives for their biological and medicinal potential remains a vibrant area of research. Molecular docking serves as a computationally efficient approach for predicting how small molecules orient and interact within a protein's binding site, making it a valuable tool in structure-based drug discovery[6,7]. The *M. tuberculosis* PknG enzyme has been reported to mediate atypical ubiquitination processes that lead to the degradation of host signaling proteins such as TRAF2 and TAK1, consequently dampening innate immune defenses[8]. Therefore, targeting PknG is an important tool for development of a new effective drugs against *M. tuberculosis* resistant strains[9]. Given their diverse bioactivities, naphthoquinone derivatives represent promising structural templates for designing new agents effective against *Mycobacterium* species. This study aimed to evaluate antimycobacterial effect of naphthoquinone natural derivatives identified by GC-MS in Henna leaves against PknG enzyme by computational studies as anti-mycobacterium agents.

1. Methodology

2.1. Natural extract and chemicals:

L. inermis dried powdered leaves (50 g) were macerated with 500 mL methanol (1:10 w/v) for 72 h with occasional shaking and filtered. Extraction was repeated in triplicate and combined extracts were concentrated under reduced pressure to obtain a yield of 9.8% w/w. Lawsone (2-hydroxy-1,4-naphoquinone) and 5-hydroxy-1,4-naphthoquinone were purchased from Alfa Alesar (Ajaohnson Matthy company, USA). 2,3 dichloro-1,4-naphthoquinone, Squalene, 1,4 naphthoquinones were purchased from Sigma-Aldrich (product of Japan).

2.2. GC-MS analysis

GC-MS analysis of the prepared sample of natural extract of was carried out using a GC/MS (GC/MS-QP2010-Ultra) instrument model from the Japanese Shimadzu Company (serial number: 020525101565SA) and a capillary column (Rtx-5 ms-30 m × 0.25 mm × 0 25 µm). The sample (1 mg) of the extract was dissolved in 1 mL methanol then 1 µL was injected using a split mode (10:1). The helium, a carrier gas, was passed at a flow rate of 1.61 ml/min, and the temperature program started from 60 ˚C at a rate of 10 ˚C/min to 300 ˚C as a last temperature degree with a holding time of 5 minutes, the temperature of injection channel was a 300 ˚C, an ion source temperature was a 200 ˚C and an interface temperature was 250 ˚C. Mass spectral analysis of the extract was performed using a scan mode with a mass to charge a range of 40–500 m/z. Component identification was achieved by comparing their retention index and mass fragmentation models with those available in the library of the National Institute of Standards and Technology (NIST) mass spectral database with (>89%) matching percentage, Kovats retention index comparison, and confirmation using analytical standards for lawsone and 5-hydroxy-1,4-naphthoquinone. Semi-quantitative analysis was conducted using normalized peak area %, and lawsone represented 20.1% of the total ion chromatographic area. The results were recorded.

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2.3. Molecular Docking

Preparation of ligand compounds and target protein

Depending on the GC-MS analysis of *L. inermis* extract, the three-dimensional assembly of the five naphthoquinones were collected from the chemical entities of biological interest CheBI online database[10]. Subsequently, the ligands set have been prepared through *LigPrep* module of Schrödinger to standardize their chemical properties[11]. Three of vital mycobacterial enzymes crystal structures for *M. tuberculosis* Protein kinase G (PknG; PDB: 2PZI, chain A, 2.00 Å resolution), IspD (2-C-methyl-D-erythritol cytidylyltransferase; PDB: 2XWL, chain A, 2.30 Å resolution), and UDP-glucose-dependent glycosyltransferase (PDB: 3CKQ, chain A, 2.40 Å resolution) were downloaded from protein data Bank (PDB) online database. Co-crystallized small molecules and non-essential water molecules were removed, while catalytically relevant ions and conserved water in the binding pocket were retained. Protein structures were prepared using Schrödinger Protein Preparation Wizard (Maestro v13.4; OPLS4 force field) including: assignment of protonation states at pH 7.0 ± 0.5 using Epik, optimization of hydrogen bonding networks, addition of missing side chains and restrained minimization to 0.3 Å RMSD.

Protein-ligand docking

Ligands were obtained from PubChem and ChEBI and processed using LigPrep (pH 7.0 ± 0.5), generating possible tautomers and protonation states. Docking was performed with Glide Extra Precision (XP) mode. Docking was performed with Glide Extra Precision (XP) mode. A receptor grid was generated around the co-crystallized ligand binding site with a 20 × 20 × 20 Å grid box centered at the binding pocket centroid. Default van der Waals scaling (0.80) was applied for nonpolar atoms. Up to 10 poses per ligand were generated and ranked by XP GlideScore. The top-ranked pose was further rescored using Prime MM-GBSA (VSGB solvation model) to refine binding energy estimates. All simulations were performed on a Windows 10 workstation, Intel Core i7, 16 GB RAM. Up to 32 stereoisomers per compound were retained for docking. The targeted proteins data set contained: Protein kinase G enzyme that maintains the existence of the mycobacterium inside the host through it is interference with the host lysosomal defence mechanism[12]. UDP-Glucose specific glycosyltransferase which is an essential enzyme that participates in biosynthetic machineries of oligosaccharide and glycoconjugate sequences production of the mycobacterial cell wall[13]. IspD enzyme that mediate the alternative mevalonate synthesis pathway, and it is descending derivatives[14]. For IspD enzyme the binding pocket was not clearly defined so it has been predicted using *site map* module of Schrödinger[11]. Naphthoquinone derivatives have been tested against the three proteins using the theory of inverse docking through *glide extreprescion docking (XP)* module in Schrödinger against these enzymes[15].

Docking Validation

Docking validation was performed by re-docking the native co-crystallized ligands into the binding pockets of PknG, IspD, and UDP-glucose glycosyltransferase using the same Glide XP protocol. RMSD values between docked and experimental poses were **1.**42 Å (2PZI), 1.96 Å (2XWL), and 1.71 Å (3CKQ), confirming reliability of the docking model (acceptable threshold <2.0 Å).

2. Results and Discussion

2.1. GC-MS analysis

The results of GC-MS analysis for *L. inermis* showed the presence of lawsone and its derivatives as shown in in Table 1. The major natural derivatives identified, more than 20%, were, squalene, lawsone and coumarin carboxylic acid derivatives. Minor constituents identified about 5% were a γ-sitosterol, α-tocopherol and phytol. This GC-MS results were confirmed with previous study that identified the presence of fifty-one natural constituents in such plant including the naphthoquinone derivatives[16,17]. Retention index (RI) validation was supported by reference databases and literature values. Lawsone GC-MS has been previously detected in henna treated samples[18].

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Table 1: GC–MS identified compounds in *L. inermis* methanolic extract.

No	IUPAC Name	Retention Time (Min)	Molecular Weight (g/mol)	Molecular Formula	Peak Area (%)
1	2-Hydroxy-1,4-naphthalenedione (Lawsone)	12.707	174	$C_{10}H_6O_3$	20.185
2	2H-1-Benzopyran-3-carboxylic acid, 2-oxo-, methyl ester **(Coumarin-3-carboxylic acid, methyl ester)**	14.647	204	$C_{11}H_8O_4$	5.131
3	3,7,11,15-Tetramethyl-2-hexadecen-1-ol **(Phytol)**	16.049	296	$C_{20}H_{40}O$	4.991
4	Coumarin-4-carboxylic acid, methyl ester	16.606	204	$C_{11}H_8O_4$	23.328
5	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-(**Squalene)**	29.611	410	$C_{30}H_{50}$	34.433
6	**dl-α-Tocopherol**	33.592	430	$C_{29}H_{50}O_2$	5.985
7	**γ-Sitosterol**	35.922	414	$C_{29}H_{50}O$	5.947

2.2. Molecular Docking

Molecular docking is a key computational perspective for identifying the binding affinity of a ligand or compound and a target or receptor[19]. This method provides admired insights for derivatives interactions with a target and affect bacterial cellular processes. In this study, the antimycobacterial of naphthoquinone derivatives through molecular simulation has showed great perceptions for their chemical reactivity and stability. Naphthoquinone, 5-Hydroxy-1,4-naphthoquinone, 2-Amino-3-chloro-1,4-naphthoquinone and Coumarin-3-carboxylic acid have shown considerable interactions with Protein kinase G enzyme with docking scores less than (-6.0) as shown in Table 2. The three former compounds interact through H-bond formation with valine 235 residue of the binding pocket while Coumarin-3-carboxylic acid interact with residue Lys 181 and GLU 280 in the presence of water (Figure 1).

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Table 2: Docking scores and binding free energies of selected ligands.

	3CKQ	2XWL	2PZI
	Docking scores (kcal·mol^{-1})	*Docking scores (kcal·mol^{-1})*	*Docking scores (kcal·mol^{-1})*
Naphthoquinone	-4.468	-3.431	**-7.571**
2-Hydroxy-1,4-naphthalenedione (Lawsone)	-5.596	**-6.025**	-5.295
5-Hydroxy-1,4-naphthoquinone	-4.468	**-6.438**	**-8.224**
2-Amino-3-chloro-1,4-naphthoquinone	-4.514	-3.355	**-7.950**
Coumarin-3-carboxylic acid	**-6.278**	**-12.501**	-6.927

3CKQ: UDP-glucose-specific glycosyltransferase (UGT), 2XWL: IspD enzyme, 2PZI, Protein kinase G (PknG)

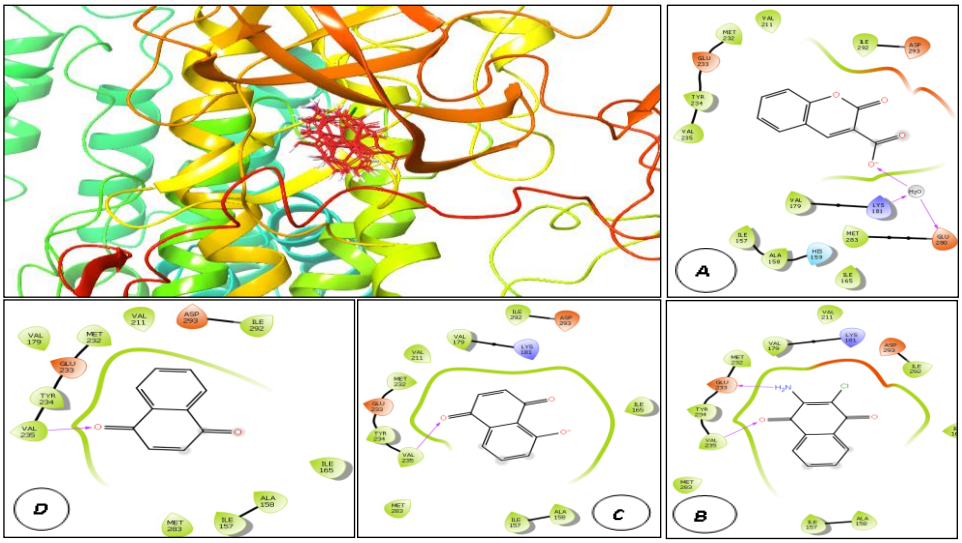

Figure 1: The interactions between naphthoquinones and Protein kinase G (pdb ID: 2PZI). A: Shows Coumarin-3-carboxylic acid interactions, B: represents 2-Amino-3-chloro-1,4 Naphthoquinone, C: 5-Hydroxy-1,4-naphthoquinone interaction, D: highlights the parent Naphthoquinone interaction with 2PZI.

Coumarin-3-carboxylic acid exerted the best interaction in comparison with the total set with docking score **-12.501** when tested against IspD enzyme**.** 2-Hydroxy-1,4-naphthalenedione and 5-Hydroxy-1,4-naphthoquinone also exhibited mild interaction with this target in their ionic state (Figure 2). Coumarin-3-carboxylic acid demonstrated a stronger predicted interaction with PknG (−12.5 kcal·mol^{-1}) than the positive reference inhibitor (−13.2 kcal·mol^{-1}), indicating potential inhibitory relevance within the validated scoring threshold.

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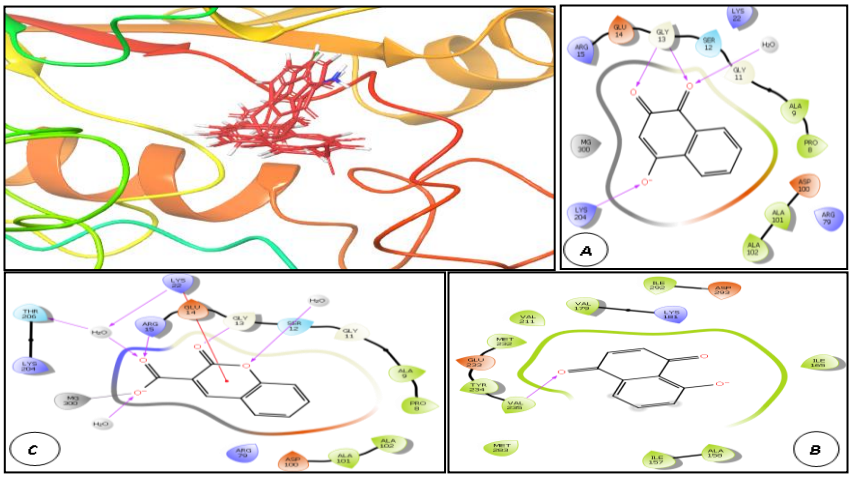

Figure 2*: The predicted interactions from XP docking of Naphthoquinones data set with IspD enzyme (pdb ID:2XWI). **A**: Interaction of 2-Hydroxy-1,4-naphthalenedione. B: Interaction of 5-Hydroxy-1,4-naphthoquinone. C: Shows the interactions Coumarin-3-carboxylic acid.*

In docking of naphthoquinone versus UDP-glucose-specific glycosyltransferase, coumarin-3-carboxylic acid showed better interaction with respect to the rest compounds as shown in Figure 3. These findings are in accordance with the results which were indicated that naphthoquinone derivatives have effects on many clinical drug resistant bacterial stains[20,21].

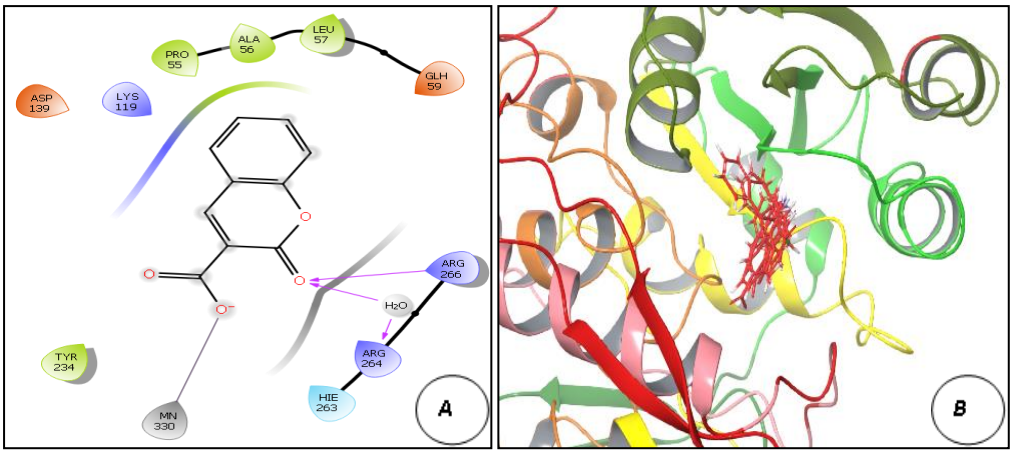

Figure 3: *A: Illustration of the interaction between Coumarin-3-carboxylic acid and UDP-glucose-specific glycosyltransferase (pdb ID:3CKQ). B: shows the different docking poses for naphthoquinone library with UDP-glucose-specific glycosyltransferase enzyme.*

3. Conclusion

This study concluded that computational study of natural naphthoquinone derivatives identified in *L. inermis* was recognised their medicinal value as antibacterial agents, emphasizing on their interactions with mycobacterium protein kinase G enzyme. The molecular docking study revealed a significant binding affinity of five naphthoquinone derivatives target protein. This underscores Coumarin-3-carboxylic acid exerted the most power interaction. All derivatives suit considerable drug-basis interaction, exhibiting antituberculosis via computational assessments. This study predicts favourable binding interactions between naphthoquinone derivatives identified from *L.*

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inermis and key *M. tuberculosis* target enzymes. These findings provide a hypothesis-generating basis for future experimental evaluation. Further in vitro and in vivo validation is required to confirm their potential antimycobacterial effects.

Abbreviations and Acronyms

NQs: Naphthoquinones.

PDB: Protein data Bank.

PknG or 2PZI: Protein kinase G.

TRAF2: Tumor necrosis factor receptor-associated factor 2.

TAK1: TGF-β-activated kinase 1.

GC-MS: Gas Chromatography–Mass Spectrometry.

NIST: National Institute of Standards and Technology.

CheBI: Chemical Entities of Biological Interest.

IspD or 2XWL: 2-C-Methyl-D-erythritol-4-phosphate cytidyltransferase.

XP: glide extreprescion docking.

3CKQ: UDP-Glucose specific glycosyltransferase.

RI: Retention index

ETHICAL STATEMENT

Not Applicable

CONFLICT OF INTEREST

No conflict of interest.

AUTHORS' CONTRIBUTIONS

All authors contributed equally, Anwar M. Abdelrahman carried out extraction and compound identification; Mohammed A. Almogaddam performed the molecular docking, Abdelgadir A. Abdelgadir carried out data analysis and wrote the manuscript draft. All authors approved the final version.

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