Theoretical Evaluation of Potential Anti-Alanine Dehydrogenase Activities of Acetamide Derivatives

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Received: 5.10.2021; Revised: 2.11.2021; Accepted: 5.11.2021; Published: 25.11.2021

Abstract: Tuberculosis is an airborne communicable syndrome, which has been observed to be among the top ten (10) causes of death worldwide. This work studied eleven molecular compounds via quantum chemical calculations, molecular docking method, and ADMET (absorption, distribution, metabolism, excretion, and toxicity). The selected obtained descriptors (Log P, HBA, HBD, and molecular weight) showed that the studied compounds have the ability to act drug-like. Compound D inhibited far better than the other studied ligands as well as the standard. ADMET properties of compound D proved that the predicted ADMET level was closer to the ADMET properties of the referenced drug (Isoniazid).

Keywords: 2-(quinoline-4-yl)oxyacetamide; tuberculosis; QSAR; DFT; docking; ADMET.

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1. Introduction

*M. tuberculosis* remains one of the dangerous diseases among human beings. Despite the continuous effort put in place by several researchers to combat this disease, the rate of killing human beings remains high. According to the report by Law et al., 2019 [1], the call for more and effective anti-tubercular drugs has increased despite several anti-tubercular drugs circulating globally. In 2019, more than 1 million tuberculosis-based death cases were reported by the world health organization (WHO), and the resistance of some of its strains to drugs remains a difficult issue in the medical world [2]. According to Kenia et al., 2016, less than half of the world's population has either latent or dormant type of tuberculosis [3].

Series of heterocyclic compounds have been observed to possess antimicrobial activities, and some of the compounds have been found to be located in natural and synthetic molecules with therapeutic values [4]. Heterocyclic ring systems are contained in many dye compounds, drug-like compounds, and several natural molecules like hormones, amino acids, and alkaloids. Many heterocyclic molecular compounds such as pyrimidines, thiazole, piperidine, pyridine, furan, pyrrolidine, and thiophene reveal substantial biological activities. According to several researchers, quinoline-based drug-like compounds have been reported to have great attention by scientists due to pharmacological importance such as antimicrobial, anti-inflammatory, antimalarial, anticancer, antiviral, and antifungal activities [5].
The role played by the quantum chemical method in the scientific sphere cannot be overemphasized. It helps in sustainability, determination of chemical structure, and elucidation of molecular reactivity [6]. Also, density functional theory remains a vital instrument for making a novel series of reasons vindicating the employed active site in the receptor residues involved in the interaction and the types of interactions further processing dehydrogenase alanine dehydrogenase methylquinolinyl (quinoline bond donor and hydrogen bond acceptor) that describe antimicrobial activities via quantum chemical calculations [16].

Molecular docking study is an emerging imperative technique used for drug development, and it remains the main tool in computer-based drug design [11]. Docking acts as a screening tool in drug discovery to identify compounds with better inhibiting affinity. It also exposes the ligand pose in the receptor's active site, which is imperative for optimization [12-15].

In this work, eleven molecular compounds were studied to identify the descriptors responsible for its anti-tubercular activities and development of a reliable quantitative structure-activity relationship (QSAR) model for better prediction of the experimental inhibition concentration (IC$_{50}$) as well as observing the interactions between the acetamide derivatives and Alanine Dehydrogenase (PDB ID: 2voe).

2. Materials and Methods

2.1. Optimization of the studied compounds.

Eleven molecular compounds synthesized by Ana et al., 2020 were optimized using quantum chemical calculations [16] via Spartan 14 software [17-25] which brought about electronic descriptors (Highest occupied molecular orbital energy, lowest unoccupied molecular orbital energy, band gap, dipole moment, log P, ovality, polarizability, hydrogen bond donor and hydrogen bond acceptor) that describe anti-tubercular activities of 2-(quinoline-4-yloxy) acetamide derivatives. The studied alkaloids were 2-((6-Methoxy-2-methylquinolin-4-yl)oxy)-1-phenylethan-1-one (A), 2-((6-Methoxy-2-methylquinolin-4-yl)oxy)-1-(4-methoxyphenyl)ethan-1-one (B), 2-((6-Methoxy-2-methylquinolin-4-yl)oxy)-1-(3-methoxyphenyl)ethan-1-one (C), 2-((6-Methoxy-2-methylquinolin-4-yl)oxy)-1-(2-methoxyphenyl)ethan-1-one (D), 2-((6-Methoxy-2-methylquinolin-4-yl)oxy)-1-(p-tolyl)ethan-1-one (E), 1-(4-Fluorophenyl)-2-((6-methoxy-2-methylquinolin-4-yl)oxy)ethan-1-one (F), 1-(4-Chlorophenyl)-2-((6-methoxy-2-methylquinolin-4-yl)oxy)ethan-1-one (G), 1-(3-Chlorophenyl)-2-((6-methoxy-2-methylquinolin-4-yl)oxy)ethan-1-one (H), 1-(3,4-Dichlorophenyl)-2-((6-methoxy-2-methylquinolin-4-yl)oxy)ethan-1-one (I), 1-(4-Isobutylphenyl)-2-((6-methoxy-2-methylquinolin-4-yl)oxy)ethan-1-one (J), 2-((6-Methoxy-2-methylquinolin-4-yl)oxy)-1-phenylpropan-1-one (K) (Table 1).

2.2. Docking study.

The molecular interactions between 2-(quinoline-4-yloxy)acetamide derivatives and alanine dehydrogenase (PDB ID: 2voe) were investigated using a docking study. Alanine dehydrogenase (PDB ID: 2voe) was obtained from a protein data bank (www.rcsb.org) before further processing. A series of molecular docking software was employed to observe the residues involved in the interaction and the types of interactions between the studied complexes. The software used were PyMOL, Autodock tool 1.5.6, Autodock vina, and Discovery studio. The observed values which showed the employed active site in the receptor...
were as follows: center (X = 23.867, Y = -0.595, Z = 63.69) and size (X = 56, Y = 68, Z = 62); as well as the spacing for individual receptor was set at 1.00 Å.

2.3. Studied ADMET properties.

Absorption, distribution, metabolism, excretion, and toxicity (ADMET) of the selected compounds with the highest binding affinity and the referenced drug used were examined using online software (admetSAR) [26]. The considered ADMET factors were Blood-Brain Barrier, Human Intestinal Absorption, Caco-2 Permeability, P-glycoprotein Substrate, P-glycoprotein Inhibitor, Renal Organic Cation Transporter, Subcellular localization, CYP450 2C9 Substrate, CYP450 2D6 Substrate, CYP450 3A4 Substrate, CYP450 1A2 Inhibitor, CYP450 2C9 Inhibitor, CYP450 2D6 Inhibitor, CYP450 2C19 Inhibitor, CYP450 3A4 Inhibitor, CYP Inhibitory Promiscuity, Human Ether-a-go-go-Related Gene Inhibition, AMES Toxicity, Carcinogens, Fish Toxicity, Tetrahymena Pyriformis Toxicity, Honey Bee Toxicity, Biodegradation.

Table 1. 2D structure of the studied compounds.

| Compound | R¹ | R² |
|----------|----|----|
| A        | H  | Ph |
| B        | H  | 4-MeO-Ph |
| C        | H  | 3-MeO-Ph |
| D        | H  | 2-MeO-Ph |
| E        | H  | 4-Me-P |
| F        | H  | 4-F-P |
| G        | H  | 4-Cl-Ph |
| H        | H  | 3-Cl-P |
| I        | H  | 3,4-(Cl)₂-Ph |
| J        | H  | 4-i-Bu-Ph |
| K        | Me | Ph |

3. Results and Discussion

3.1. Calculated descriptors from optimized 2-(quinoline-4-yloxy)acetamide derivatives.

Calculated molecular descriptors for 2-(quinoline-4-yloxy)acetamide derivatives used to investigate their anti-tubercular activities were molecular weight, hydrophobicity (Log P), volume (V), Area, polar surface area (PSA), ovality, dipole moment (DM), Highest occupied molecular Orbital (E_HOMO), and Lowest unoccupied molecular orbital (E_LUMO) energies as shown in Tables 2. The calculated descriptors were subjected to Lipinski rule of five (Molecular Weight ≤ 500, HBD ≤ 5, HBA ≤ 10 and Log P ≤ 5) [27], so to examine the drug-likeness ability of the studied compounds, and it was observed that all the studied compounds conformed well with the Lipinski rule of five which is a proof that all the compounds under study potential ability to act as a drug against M. tuberculosis. The calculated molecular weight, HBD, HBA and Log P for compound A-K were 307.349 amu, 337.375 amu, 337.375 amu, 337.375 amu, 321.376 amu, 325.339 amu, 341.794 amu, 341.794 amu, 376.239 amu, 363.457 amu.
am and 321.376; 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0; 4, 5, 5, 4, 4, 4, 4, 4, 4 and 0.18, 0.05, 0.05, 0.05, 0.66, 0.33, 0.73, 0.73, 1.29, 1.83, 0.67 (Table 2).

The residues involved in each interaction were Ala179, Val239, Leu240, Leu130, Leu127, Pro242 for compound A; Gly125, Ala126, Leu240, Gly177, Ala179, Ser134, Leu130, Ala131 for compound B; His96, Asp270, Gln99, Lys10, Ala299 for compound C; His96, Leu130, Ala131, Ser134 for compound D; Ala137, Ser134, Leu130, Leu240, Lys75, Pro302, Phe94, Met133 for compound E; Leu240, Val239, Ala179, Gly177, Leu127, Pro242, Asp198 for compound F; Tyr147, His148, Tyr283 for compound G; Ala179, Gly177, Val239, Leu240, Pro242, Leu127, Leu130 for compound H; Tyr147, His148 for the compound I; Tyr147, His148, Gln143, Tyr283, Phe14 for compound J; Tyr283, Ser304, Leu140, Val144, His148, Tyr147 for compound K. In this work, the combination of interactions observed between compound D and 2voe were Conventional Hydrogen Bond, Alkyl, Pi-Alkyl, Pi-Sigma. These proved to have enhanced its ability to bind well to the studied receptor than other studied compounds (Figure 1).
### Table 3. Interactions between 2-(quinoline-4-yloxy)acetamide derivatives and Alanine Dehydrogenase (PDB ID: 2voe).

| Binding Affinity (kcal/mol) | Residue Involved in the interaction | Types of Interaction |
|-----------------------------|------------------------------------|----------------------|
| A -6.5                      | Ala179, Val239, Leu240, Leu130, Leu127, Pro242 | Conventional Hydrogen Bond, Pi-Alkyl, Alkyl |
| B -7.1                      | Gly125, Ala126, Leu240, Gly177, Ala179, Ser134, Leu130, Ala131 | Conventional Hydrogen Bond, Amide-Pi Stacked, Alkyl, Pi-Alkyl |
| C -6.2                      | His96, Asp270, Gln99, Lys10, Ala299, | Conventional Hydrogen Bond, Carbon Hydrogen Bond, Pi-Anion, Pi-Donor Hydrogen Bond, Pi-Sigma, Pi-Alkyl |
| D -7.7                      | His96, Leu130, Ala131, Ser134 | Conventional Hydrogen Bond, Alkyl, Pi-Alkyl, Pi-Sigma |
| E -7.4                      | Ala137, Ser134, Leu130, Leu240, Lys75, Pro302, Phe94, Met133 | Unfavorable Acceptor-Acceptor, Pi-Cation, Pi-Sigma, Pi-Pi T-shaped, Alkyl, Pi-Alkyl |
| F -6.7                      | Leu240, Val239, Ala179, Gly177, Leu127, Pro242, Asp198 | Carbon Hydrogen Bond, Halogen, Alkyl, Pi-Alkyl, Pi-Sigma |
| G -6.5                      | Tyr147, His148, Tyr283 | Conventional Hydrogen Bond, Pi-Alkyl |
| H -6.8                      | Ala179, Gly177, Val239, Leu240, Pro242, Leu127, Leu130 | Conventional Hydrogen Bond, Alkyl, Pi-Alkyl, Pi-Sigma |
| I -6.6                      | Tyr147, His148 | Conventional Hydrogen Bond, Pi-Pi Stacked |
| J -7.0                      | Tyr147, His148, Gln143, Tyr283, Phe14 | Conventional Hydrogen Bond, Carbon Hydrogen Bond, Pi-Pi Stacked, Pi-Alkyl |
| K -6.3                      | Tyr283, Ser304, Leu140, Val144, His148, Tyr147 | Conventional Hydrogen Bond, Carbon Hydrogen Bond, Pi-Pi Stacked, Alkyl |
| INH -5.3                    | Note: INH denotes Isoniazid (Reference Drug) |

#### Figure 1. Bonded and non-bonded interactions of D against Alanine Dehydrogenase (PDB ID: 2voe).

#### 3.3. ADMET properties of studied selected compounds.

The ADMET report for the selected compound D and the referenced drug (Isoniazid) are shown in Table 4. Absorption, distribution, metabolism, excretion, and toxicity for...
compound D with better binding affinity than other studied compounds were calculated using the admetSAR1 server. The compound with higher human intestinal absorption values is expected to have a higher ability to be absorbed well [28-32]. Therefore, the values obtained for human intestinal absorption (HIA) for selected compounds correlated with the standard (Isoniazid), proving that the selected compounds can be absorbed in the intestine. Also, a fair correlation was observed between compound D and Isoniazid for the blood-brain barrier. As shown in Table 4, the evaluation of predicted Cytochrome P450 showed that compound D and the standard are non-inhibitors of CYP450 2C9 Inhibitor and CYP450 2D6 Inhibitor. Still, the selected compounds and the reference drug are inhibitors of CYP450 1A2 Inhibitor. Also, compound D is an inhibitor of CYP450 2C19 Inhibitor and CYP450 3A4 Inhibitor. More so, both compounds D and Isoniazid (Standard) are non-carcinogenic agents and are not readily biodegradable, as displayed in Table 4.

4. Conclusions

In this work, eleven chemical compounds were investigated via the quantum chemical method, molecular docking, and ADEMT studies. The selected obtained descriptors (Log P, HBA, HBD and molecular weight) proved the ability of the studied compounds to have drug-like properties. Molecular docking study was performed in order to identify the non-bonding interactions and calculated the binding affinity that exists between the eleven compounds and the Alanine Dehydrogenase. Compound D inhibited far better than the other studied ligands as well as the standard. ADMET properties of D proved that the predicted ADMET level was closer to the ADMET properties of the referenced drug (Isoniazid).

| Mode                                | Compound D                      | Isoniazid                      |
|-------------------------------------|---------------------------------|--------------------------------|
| Blood-Brain Barrier                 | Result: BBB+ Probability: 0.9305 | Result: BBB+ Probability: 0.9895 |
| Human Intestinal Absorption         | HIA+ Probability: 0.9926        | HIA+ Probability: 0.9892       |
| Caco-2 Permeability                 | Caco2+ Probability: 0.8120      | Caco2+ Probability: 0.6959     |
| P-glycoprotein Substrate            | Non-substrate Probability: 0.6121 | Non-substrate Probability: 0.8315 |
| P-glycoprotein Inhibitor            | Inhibitor Probability: 0.6095   | Non-inhibitor Probability: 0.9778 |
| Renal Organic Cation Transporter    | Non-inhibitor Probability: 0.7623 | Non-inhibitor Probability: 0.9054 |
| Subcellular localization            | Mitochondria Probability: 0.7309 | Mitochondria Probability: 0.7026 |
| CYP450 2C9 Substrate                | Non-substrate Probability: 0.8189 | Non-substrate Probability: 0.9088 |
| CYP450 2D6 Substrate                | Non-substrate Probability: 0.5716 | Non-substrate Probability: 0.9116 |
| CYP450 3A4 Substrate                | Substrate Probability: 0.6252   | Non-substrate Probability: 0.7557 |
| CYP450 1A2 Inhibitor                | Inhibitor Probability: 0.8975   | Inhibitor Probability: 0.6482  |
| CYP450 2C9 Inhibitor                | Non-inhibitor Probability: 0.7850 | Non-inhibitor Probability: 0.9273 |
| CYP450 2D6 Inhibitor                | Non-inhibitor Probability: 0.8230 | Non-inhibitor Probability: 0.9443 |
| CYP450 2C19 Inhibitor               | Inhibitor Probability: 0.7781   | Non-inhibitor Probability: 0.9513 |
| CYP450 3A4 Inhibitor                | Inhibitor Probability: 0.7722   | Non-inhibitor Probability: 0.5111 |
| CYP Inhibitory Promiscuity          | High CYP Inhibitory Promiscuity Probability: 0.8074 | Low CYP Inhibitory Promiscuity Probability: 0.9342 |
| Human Ether-a-go-go-Related Gene Inhibition | Weak inhibitor Probability: 0.9603 | Weak inhibitor Probability: 0.9872 |
| Carcinogens                         | Non-carcinogens Probability: 0.9470 | Non-carcinogens Probability: 0.7514 |
| Fish Toxicity                       | High FHMT Probability: 0.6835   | Low FHMT Probability: 0.9451   |
| Tetrahymanena Pyriformis Toxicity   | High TPT Probability: 0.9856    | Low TPT Probability: 0.7464    |
| Honey Bee Toxicity                  | High HBT Probability: 0.6198    | Low HBT Probability: 0.8399    |
| Biodegradation                      | Not ready biodegradable Probability: 0.8484 | Not ready biodegradable Probability: 0.9810 |
Funding

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Acknowledgments

We are grateful to the Department of Pure and Applied Chemistry, Osun State University, for the computational resources and Mrs. E.T. Oyebamiji as well as Miss Priscilla F. Oyebamiji for the assistance in the course of this study.

Conflicts of Interest

The authors declare that they have no known competing financial interests or personal relationships which have or could be perceived to have influenced the work reported in this article.

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