Data Article

Dataset on insightful bio-evaluation of 2-(quinoline-4-yloxy)acetamide analogues as potential anti-*Mycobacterium tuberculosis* catalase-peroxidase agents via *in silico* mechanisms

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**A B S T R A C T**

The continuous havoc wreaked by tuberculosis among humans worldwide remains colossal. In this work, twenty-one (21) 2-(quinoline-4-yloxy)acetamide analogues were observed against *Mycobacterium tuberculosis* catalase-peroxidase (This enzyme shields bacteria from poisonous drug-like molecules) (PDB ID: 1sj2) using density functional theory method, QSAR study using material studio software and docking method via PyMol, AutoDock Tool, AutoDock Vina and Discovery studio 2017 as well as ADMET study

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via admetSAR2. Twelve descriptors were obtained from the optimized compounds which were used to develop valid QSAR model. More so, the binding affinity between 2-(quinoline-4-yloxy)acetamide analogues and Mycobacterium tuberculosis catalase-peroxidase (PDB ID: 1sj2) via docking method were reported. ADMET properties of some selected compounds were also examined.

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### Specification Table

| Subject                  | Bioinformatics |
|--------------------------|----------------|
| Specific subject area    | Drug Discovery |
| Type of data             | Table          |
| How data were            | Spartan’14, PaDEL-Descriptors, Data_pretreatment_train_test 1.0, Dataset |
| Data format              | Raw Data       |
| Parameters for data      | B3LYP, 6-31G*; Multiple linear regression (MLR), Genetic function approximation (GFA), EduPyMOL-v1.7.4.4-Win32, biovia2019.ds2019client, mgtools_win32_1.5.6 and Autodock vina |
| Collection               | Twenty-one molecular compounds were theoretically investigated using density functional theory (DFT). The investigated compounds were divided into two sets (Training set and test set) and the descriptors from the training set were used to develop reliable QSAR model and test set used to confirm it reliability via material studio software. All compounds were docked against Mycobacterium tuberculosis catalase-peroxidase via molecular docking method and ADMET properties of the compounds with highest binding affinity was examined before interpretation of result. |
| Data source location     | Computational and Theoretical Chemistry Research Laboratory, Department of Basic Sciences, Adeleke University, Ede, Osun State, Nigeria |
| Data accessibility       | All the data [experimental [1] and predicted] can be accessed in the data article |
| Related research article | A.F. Borsoi, J.D. Paz, B.L. Abbadi, F.S. Macchi, N. Sperotto, K. Pissinate, R.S. Rambo, A.S. Ramos, D. Machado, M. Viveiros, C.V. Bizarro, L.A. Basso, P. Machado. Design, synthesis, and evaluation of new 2-(quinoline-4-yloxy)acetamide-based antituberculosis agents. Eur J Med Chem 192 (2020) 112179. |

### Value of the Data

- The calculated data (descriptors) from the optimized 2-(quinoline-4-yloxy)acetamide derivatives will help researchers to recognize descriptors which describe their inhibiting capacity.
- The selected descriptors from the optimized 2-(quinoline-4-yloxy)acetamide derivatives will also assist researchers to develop reliable and valid QSAR model with effective cytotoxicity.
- The calculated binding affinity will help scientists to locate 2-(quinoline-4-yloxy)acetamide based compound with utmost inhibiting ability against Mycobacterium tuberculosis catalase-peroxidase (PDB ID: 1sj2).
- The proposed drug-like molecules will assist researchers to have access to library of molecules with better inhibiting ability than the standard drug used in this work.
1. Data Description

Table 1 showed 2D structures of 2-(quinoline-4-yloxy)acetamide derivatives experimentally synthesised by Borsoi et al. [1] which was further converted to 3D and optimized using quantum chemical method via 6–31G* as basis set.

Table 1
3D structures of 2-(quinoline-4-yloxy)acetamide derivatives.

| R      | Proposed compound |
|--------|------------------|
| Ph     |                  |
| 3-MeO-Ph |                 |
| 3,5-(MeO)₂-Ph |           |
| 4-F-Ph   |                 |
| 3-F-Ph   |                 |
| 2-F-Ph   |                 |
| 3,4-(F)₂-Ph |             |
| 4-Cl-Ph  |                 |
| 3-Cl-Ph  |                 |
| 2-Cl-Ph  |                 |
| 3,4-(Cl)₂-Ph |           |
| 2,3-(Cl)₂-Ph |         |
| 3-Cl-4-Br-Ph |            |
| 4-Br-Ph  |                 |
| 3-Br-Ph  |                 |
| 4-F₂C-Ph |                 |
| 3-F₂C-Ph |                 |
| 4-O₂N-Ph |                 |
| 4-i-Pr-Ph |               |
| 4-t-Bu-Ph |                |
| 2-Naphthyl |              |
| P1      | CH₂₂F            |
| P2      | CH₂Cl            |
| P3      | CH₂Br            |
| P4      | CH₃              |
Table 2
Calculated QSAR model using selected descriptors from optimized 2-(quinoline-4-yloxy)acetamide derivatives.

| Equation | R² | Adj. R² | C.VR² | P-value | F-value |
|----------|----|---------|-------|---------|---------|
| IC₅₀ = 59.690892769 (E_{HOMO}) - 13.673062012(\log P) + 3.992788387(HBA) + 409.194825576 | 0.94 | 0.92 | 0.89 | P < 0.0001 | 52.26 |

Table 3
Experimental and Predicted IC₅₀ for 2-(quinoline-4-yloxy)acetamide derivatives.

|          | Experimental IC₅₀ | GFA |
|----------|------------------|-----|
| 1        | 5.6              | 7.0 |
| 2        | 32.3             | 31.3 |
| 3        | 29.5             | 18.7 |
| 4        | 16.8             | 19.3 |
| 5        | 16.8             | 18.7 |
| 6        | 19.2             | 18.1 |
| 7        | 3.9              | 17.1 |
| 8        | 15.9             | 12.0 |
| 9        | 7.9              | 12.0 |
| 10       | 18.8             | 12.6 |
| 11       | 0.3              | 3.1 |
| 12       | 28.7             | 4.3 |
| 13       | 1.6              | -0.4 |
| 14       | 13.9             | 8.3 |
| 15       | 13.9             | 7.7 |
| 16       | 7.2              | 8.7 |
| 17       | 7.2              | 7.5 |
| 18       | 30.8             | 31.1 |
| 19       | 1.9              | 3.9 |
| 20       | 3.7              | -1.8 |
| 21       | 7.6              | 8.1 |

* Test Set

As shown in Table S1, twelve descriptors were obtained from the optimized 2-(quinoline-4-yloxy)acetamide derivatives and further screened for anti-tuberculosis activity. The descriptors obtained were highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), band gap, dipole moment, molecular weight, area, volume, ovality, lipophilicity (Log P), polarizability, hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA) and the screened descriptors were also used for further analysis.

Table 2 displays the developed quantitative structure-activity relationship (QSAR) model using selected descriptors obtained from the optimized 2-(quinoline-4-yloxy)acetamide derivatives via series of software (Dataset Division GUI 1.2 software [2,3] and material studio software [4]). The descriptors involved in the developed QSAR model were E_{HOMO}, Log P and HBA and the statistical factors considered for QSAR validation were adjusted squared correlation coefficient (Adj R²) (0.92), cross validation correlation coefficient (C.VR²) (0.89), P-Value (P < 0.0001) and F-Value (52.26). The predicted inhibition concentration (IC₅₀) using the developed model were displayed in Table 3.

The binding affinity obtained between the optimized 2-(quinoline-4-yloxy)acetamide derivatives and Mycobacterium tuberculosis catalase-peroxidase (PDB ID: 1sj2 [5]) were reported in Table 4. The calculated binding affinity for compound 1–21 were −10.1 kcal/mol, −8.2 kcal/mol, −7.8 kcal/mol, −8.2 kcal/mol, −10.9 kcal/mol, −8.5 kcal/mol, −11.3 kcal/mol, −8.4 kcal/mol, −10.5 kcal/mol, −7.9 kcal/mol, −11.4 kcal/mol, −7.5 kcal/mol, −8.5 kcal/mol, −7.5 kcal/mol, −10.4 kcal/mol, −9.2 kcal/mol, −8.9 kcal/mol, −7.9 kcal/mol, −7.4 kcal/mol, −8.0 kcal/mol and −11.2 kcal/mol and compared to the calculated binding affinity for the standard (Isoniazid) −6.0 kcal/mol. Four molecular compounds were also predicted and docked against Mycobacterium
### Table 4
Calculated scoring, residues and types of non-bonding interactions.

|       | Binding Affinity (kcal/mol) | Residues involved in the interactions | Types of Non-bonding interaction involved |
|-------|-----------------------------|---------------------------------------|------------------------------------------|
| 1.    | -10.1                       | Ile103, His270, Arg104, Trp107,      | Van der waals, Carbon Hydrogen Bond,     |
|       |                              | Ile266, Leu265                          | Pi-Cation, Pi-Pi Stacked, Pi-Pi T-shaped,|
|       |                              |                                        | Amide-Pi Stacked, Alkyl, Pi-Alkyl        |
| 2.    | -8.2                        | Ala478, Leu514, Arg595, Arg640, Asp511| Conventional Hydrogen bond, Anion, Alkyl,|
|       |                              |                                        | Pi-Alkyl                                  |
| 3.    | -7.8                        | Arg595, Asp511, Arg640, Leu514         | Pi-Anion, Alkyl, Pi-Alkyl                 |
| 4.    | -8.2                        | Arg640, Lys639, Ser474, Leu514, Ala478| Conventional Hydrogen bond, Halogen      |
|       |                              |                                        | (Fluorine), Pi-Alkyl                      |
| 5.    | -10.9                       | Leu265, Trp107, Ile266, Phe252,       | Halogen (Fluorine), Alkyl, Pi-Alkyl,     |
|       |                              | Trp321, Ile103, Gly269, Pro100, Arg104| Amide-Pi Stacked, Pi-Pi T-shaped, Pi-Pi   |
| 6.    | -8.5                        | Ala478, Arg595, Leu514, Lys639,       | Conventional Hydrogen bond, Halogen      |
|       |                              | Asp509, Arg640                          | (Fluorine), Alkyl, Pi-Alkyl               |
| 7.    | -11.3                       | Ile266, Trp107, Phe252, Leu265, Ile103,| Conventional Hydrogen bond, Halogen      |
|       |                              | Gly269, Gly273, Pro100, Phe272, Arg104| (Fluorine), Pi-Pi Stacked, Amide-Pi Stacked, Alkyl, Pi-Alkyl |
| 8.    | -8.4                        | Leu514, Arg595, Arg640, Ala478         | Conventional Hydrogen bond, Alkyl, Pi-Alkyl |
| 9.    | -10.5                       | Trp321, His270, Arg104, Ile266, Phe252,| Conventional Hydrogen bond, Pi-Cation,   |
|       |                              | Trp107, Leu265                          | Pi-Sigma, Pi-Pi Stacked, Pi-Pi T-shaped, Amide-Pi Stacked, Alkyl, Pi-Alkyl |
| 10.   | -7.9                        | Lys613, Ala591, Asp612, His116,       | Conventional Hydrogen bond, Pi-Cation,   |
|       |                              | Lys590, Leu616, Pro603                 | Pi-Anion, Alkyl, Pi-Alkyl                 |
| 11.   | -11.4                       | Ile266, Trp107, Phe252, Ile103, Leu265,| Pi-Pi Stacked, Pi-Pi T-shaped, Amide-Pi Stacked, Alkyl, Pi-Alkyl |
|       |                              | Trp321, Pro100, Arg104                 |                                            |
| 12.   | -7.5                        | Arg640, Ser474, Asp513, Lys639         | Conventional Hydrogen bond, Carbon Hydrogen bond, Pi-Donor Hydrogen Bond, Alkyl, Pi-Alkyl |
| 13.   | -8.5                        | Arg59, Tyr63                            | Conventional Hydrogen bond, Pi-Alkyl     |
| 14.   | -7.5                        | Asp194, Gly120, Trp198, Asp194         | Pi-Anion, Amide-Pi Stacked, Pi-Alkyl, Pi-Anion, Carbon Hydrogen Bond, Pi-Pi Stacked, Pi-Pi T-shaped, Amide-Pi Stacked, Alkyl, Pi-Alkyl |
| 15.   | -10.4                       | Trp107, Leu265, Trp412, Leu415,       |                                            |
|       |                              | His270, Arg104, Trp321, Ile103, Ile266|                                            |
| 16.   | -9.2                        | Thr475, Leu514, Ala478, Lys639,       | Van der waals, Carbon Hydrogen Bond,     |
|       |                              | Ile497, Val517, Val507, Ser474,       | Halogen (Fluorine), Amide-Pi Stacked,    |
|       |                              | Arg640, Asp513                          | Alkyl, Pi-Alkyl                           |
| 17.   | -8.9                        | Ala478, Arg595, Leu514, Tyr638,       | Conventional Hydrogen bond,              |
|       |                              | Lys639, Asp511, Asp509, Arg640         | Halogen (Fluorine), Pi-Anion, Alkyl, Pi-Alkyl |
| 18.   | -7.9                        | Leu616, Ala591, Asp612, Lys613,       | Conventional Hydrogen bond, Carbon Hydrogen bond, Pi-Cation, Pi-Anion, Alkyl, Pi-Alkyl |
|       |                              | Lys590, His116, Pro219                | Pi-Anion, Pi-Donor Hydrogen Bond, Amide-Pi Stacked, Alkyl, Pi-Alkyl |
| 19.   | -7.4                        | Val196, Gly120, Met126, Asp194,       | Conventional Hydrogen bond,              |
|       |                              | Trp198, Arg119                          | Halogen (Fluorine), Pi-Anion, Alkyl, Pi-Alkyl |
| 20.   | -8.0                        | Leu514, Arg595, Ala478, Arg640,       | Conventional Hydrogen bond, Alkyl, Pi-Alkyl |
|       |                              | Tyr638                                 |                                            |
| 21.   | -11.2                       | Trp107, Ile103, His270, Arg104,       | Conventional Hydrogen bond, Pi-Cation,   |
|       |                              | His108                                 | Pi-Sigma, Pi-Pi T-shaped, Amide-Pi Stacked, Pi-Alkyl |
| INH   | -6.0                        | -                                     | -                                        |

**Predicted Compounds**

|       |                             |                                    |
|-------|------------------------------|-----------------------------------|
| P1    | -8.2                        | Arg104, Gly269, Phe272, Trp-107,  |
|       |                              | Ile266                            |
| P2    | -7.6                        | Lys693, Leu514, Ile497, Ala478,   |
|       |                              | Arg595, Asn508                      |
| P3    | -7.7                        | Leu265, Trp107, Gly269, Leu415,   |
|       |                              | Trp412, His270, Arg104             |
| P4    | -7.7                        | Arg104, Pro100, Gly269, Trp107,   |
|       |                              | Phe252, Ile266                      |

INH = Isoniazid
Fig. 1. Residual interactions between compound 11 and *Mycobacterium tuberculosis* catalase-peroxidase (PDB ID: 1sj2).

Fig. 2. Residual interactions between compound P1 and *Mycobacterium tuberculosis* catalase-peroxidase (PDB ID: 1sj2).

*tuberculosis* catalase-peroxidase (PDB ID: 1sj2) and their calculated binding affinity were compared to calculated binding affinity for Isoniazid (Table 4). The amino acid residues involved in the interaction between compound 11 as well as P1 and *Mycobacterium tuberculosis* catalase-peroxidase were displayed in Figs. 1 and 2.
Table 5 shows the Lipinski rule of five for compounds with highest calculated binding affinity (Compound 11 and P1 (from the proposed compounds). The calculated factors considered for the Lipinski rule of five were molecular weight \( \leq 500 \text{ amu} \), AlogP \( \leq 5 \), H-bond acceptor \( \leq 10 \), h-bond donor \( \leq 5 \), rotatable bonds \( \leq 5 \). Also, the selected compounds (Compound 11 and P1) were subjected to adsorption, distribution, metabolism, excretion and toxicity analysis (ADMET) using admetserver 2 server (S2).

2. Experimental Design, Materials and Methods

Twenty-one molecular compounds were optimized using density functional theory via Spartan 14 software [6]. In density functional theory method, three-parameter density functional which includes Becke’s gradient exchange correction [7] and the Lee, Yang, Parr correlation functional. As reported by Semire et al., (2017) [8], exactness of density functional theory (DFT) method is a function of the selected basis set; therefore, 6-31G* was used for optimization of the investigated drug-like molecules. The examined 2-(quinoline-4-yloxy)acetamide derivatives were:

- 4-(Benzyl oxy)-6-methoxy-2-methylquinoline (1),
- 6-Methoxy-4-(3-methoxybenzyl)oxy)-2-methylquinoline (2),
- 4-(3,5-Dimethoxybenzyl)oxy)-6-methoxy-2-Methylquinoline (3),
- 4-((4-Fluorobenzyl)oxy)-6-methoxy-2-methylquinoline (4),
- 4-(3-Fluorobenzyl)oxy)-6-methoxy-2-methylquinoline (5),
- 4-(2-Fluorobenzyl)oxy)-6-methoxy-2-methylquinoline (6),
- 4-(3,4-Difluorobenzyl)oxy)-6-methoxy-2-methylquinoline (7),
- 4-(4-Chlorobenzyl)oxy)-6-methoxy-2-methylquinoline (8),
- 4-((3-Chlorobenzyl)oxy)-6-methoxy-2-methylquinoline (9),
- 4-(2-Chlorobenzyl)oxy)-6-methoxy-2-methylquinoline (10),
- 4-(3,4-Dichlorobenzyl)oxy)-6-methoxy-2-methylquinoline (11),
- 4-(2,3-Dichlorobenzyl)oxy)-6-methoxy-2-methylquinoline (12),
- 4-(4-Bromo-3-chlorobenzyl)oxy)-6-methoxy-2-Methylquinoline (13),
- 4-(4-Bromobenzyl)oxy)-6-methoxy-2-methylquinoline (14),
- 4-(4-Bromobenzyl)oxy)-6-methoxy-2-methylquinoline (15),
- 6-Methoxy-2-methyl-4-((4-(trifluoromethyl)benzyl)oxy)Quinolone (16),
- 6-Methoxy-2-methyl-4-((3-(trifluoromethyl)benzyl)oxy)Quinolone (17),
- 6-Methoxy-2-methyl-4-((4-nitrobenzyl)oxy)quinolone (18),
- 4-(3-Isopropylbenzyl)oxy)-6-methoxy-2-methylquinoline (19),
- 4-(4-(Tert-butyl)benzyl)oxy)-6-methoxy-2-methylquinoline (20),
- 6-Methoxy-2-methyl-4-(naphthalen-2-ylmethoxy)quinolone (21).

The examined compounds were divided into two (training set and test set) and the descriptors from the training set compounds were used to developed reliable QSAR model whereas the test set was used to validate the predicting capacity of the developed QSAR model. In this work, four statistical factors (adjusted squared correlation coefficient (Adj.R²), cross validation squared correlation coefficient (C.VR²), F-value and P-value) were considered for QSAR validation. All the
compounds investigated in this work were docked against *Mycobacterium tuberculosis* catalase-peroxidase (PDB ID: 1sj2) using series of software. The downloaded *Mycobacterium tuberculosis* catalase-peroxidase from protein data bank (www.rcsb.org) was subjected to PyMOL software so as to remove non-amino acid material before locating active site for docking calculation using autodock tool and autodock vina 1.1.2 respectively. The calculated grid box to identify the binding site for *Mycobacterium tuberculosis* catalase-peroxidase (PDB ID: 1sj2) was as follows: center \((X = 39.493, Y = 5.682, Z = 43.68)\) and size \((X = 24, Y = 32, Z = 116)\), the spacing was set to be 1.00Å and the exhaustiveness was set at default (8) (Fig. 3).

**Ethics Statement**

Not applicable.

**Declaration of Competing 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.

**CRediT Author Statement**

Abel Kolawole Oyebamiji: Conceptualization, Methodology, Writing – original draft; Olubunmi Modupe Josiah: Data curation; Sunday Adewale Akintelu: Software, Visualization; Moriam Dasola Adeoye: Data curation; Babatunde Olasupo Sabitu: Writing – review & editing; Dayo Felix Latona: Writing – review & editing; Akintomiwa O. Esan: Writing – review & editing; Emmanuel Ayodele Soetan: Software, Visualization; Banjo Semire: Supervision, Software, Validation.

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**Supplementary Materials**

Supplementary material associated with this article can be found in the online version at doi:10.1016/j.dib.2021.107441.

**References**

[1] A.F. Borsoi, J.D. Paz, B.L. Abbadi, F.S. Macchi, N. Sperotto, K. Pissinate, R.S. Rambo, A.S. Ramos, D. Machado, M. Viveiros, C.V. Bizarro, L.A. Basso, P. Machado, Design, synthesis, and evaluation of new 2-(quinoline-4-yloxy)acetamide-based antituberculosis agents, Eur. J. Med. Chem. 192 (2020) 112179.

[2] S.B. Olasupo, A. Uzairu, G. Shallangwa, S. Uba, Quantitative structure-activity relationship (QSAR) studies and molecular docking simulation of norepinephrine transporter (NET) inhibitors as anti-psychotic therapeutic agents, J. Turk. Chem. Soc. Sect. A Chem. 7 (1) (2019) 179–196.

[3] B.O. Sabitu, U. Adamu, G.A. Shallangwa, S. Uba, Computer-aided drug design and in silico pharmacokinetics predictions of some potential antipsychotic agents, Sci. Afr. 12 (2021) e00734.

[4] A.K. Oyebamiji, S.A. Akintelu, O.P. Amao, M.O. Kaka, A.E. Morakinyo, F.A. Amao, B. Semire, Dataset on theoretical bio-evaluation of 1,2,4-thiadiazole-1,2,4-triazole analogues against epidermal growth factor receptor kinase down regulating human lung cancer, Data Brief 37 (2021) 107234.

[5] T. Bertrand, N.A.J. Eady, J.N. Jones, J.M. Nagy Jesmin, B. Jamart-Grégoire§, E.L. Raven, K.A. Brown, Crystal structure of Mycobacterium tuberculosis catalase-peroxidase, J. Biol. Chem. 279 (37) (2004) 38991–38999.

[6] A.K. Oyebamiji, O.A. Fadare, B. Semire, Anti-gastric cancer activity of 1,2,3-triazolo[4,5-d]pyrimidine hybrids (1,2,3-TPH): QSAR and molecular docking approaches, Heliyon 6 (2020) e03561.

[7] A.D. Becke, Density functional thermochemistry. III. The role of exact exchange, J. Phys. Chem. 98 (1993) 5648–5652.

[8] B. Semire, A.K. Oyebamiji, O.A. Odunola, Tailoring of energy levels in (2Z)-2-cyano-2-[2-[(E)-2-[(E)-2-(p-tolyl)vinyl]thieno[3,2-b]thiophen-5-yl]vinyl]pyran-4-ylidene]acetic acid derivatives via conjugate bridge and fluorination of acceptor units for effective D–p–A dye-sensitized solar cells: DFT–TDDFT approach, Res. Chem. Intermed. 43 (2017) 1863–1879.