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ORIGINAL RESEARCH ARTICLE

Computational Analysis of the Impact of Environmental Pollutants on Arginine-Rich Catalase Enzyme

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ABSTRACT

Background: Molecular docking is a computational tool widely used to investigate protein–ligand interactions and assess the potential molecular effects of environmental pollutants. As an example, nitric acid (HNO_3) is a major component of acid rain, and it poses serious risks to enzymes (cellular signalling) and antioxidants such as catalase.

Objectives: We aimed to study how HNO_3 interacts with catalase, which is found in some bacteria and other living cells, via the development of HNO_3 as a synthetic ligand and the determination of the binding interface characterized by a binding pocket dense in arginine residues.

Methods: Using AutoDock Vina as well as downstream visualization software, we were able to map out the binding site and characterize any hydrogen bonds, salt bridges, and electrostatic interactions observed within the binding interface. Catalase from Penicillium vitale (PDB ID: 1DGB) was used as the receptor.

Results: Based upon our binding analysis, we found HNO_3 (as a synthetically developed ligand) has many polar contacts and forms strong anchors through several high-affinity polar contacts predominantly with ARG A:365 and ARG A:72. However, there are also significant areas of electrostatic repulsion between adjacent positively charged arginine residues on catalase, suggesting a mechanism of inhibition. The receptor's stereochemistry has been validated through Ramachandran plotting, validating its requisite structure for docking studies.

Conclusion: The results further our understanding of ligand-modulated functioning via arginine-based binding domains and provide molecular support for the ligand's role as an inhibitor. The docking analysis demonstrated that nitric acid was successfully accommodated within the catalytic pocket of catalase. The best-ranked binding pose exhibited a binding affinity of -3.9 kcal/mol, indicating a favorable interaction between the ligand and the receptor. This docking pose was selected for subsequent interaction analysis because it presented the lowest predicted binding free energy together with the most stable orientation within the active site.

Keywords: **Molecular docking; catalase receptor; arginine cluster; AutoDock Vina; electrostatic repulsion**

1. INTRODUCTION

Acid Rain, which contains a high concentration of Nitric Acid (HNO3), significantly threatens cellular enzymes, specifically an important antioxidant, Arginine-Rich Catalase. Catalase is an enzyme that has both a heme component and is found throughout aerobic organisms, including the human liver, erythrocytes, and all epithelial tissue. It exhibits its most prominent role in detoxifying hydrogen peroxide (H2O2) converted to water and oxygen thus providing protection against oxidative

cellular deterioration [1]. From molecular docking simulations, there appears to be an ability of HNO3 to interact with the active site of Catalase via either direct hydrogen bonding or through the possible involvement of electrostatic interference with the heme-binding pocket or the adjacent arginine & histidine residues, altering the geometric form of the Catalytic site thus reducing the capacity of the enzyme to perform enzymatic activities [2]

Environmental toxicity of acid rain and computational toxicology: computer-based methods like molecular docking enable researchers to determine how well a small molecule will fit into and interact with protein active sites. Homologous proteins good targets for finding new therapies because of their role in cell signaling, replicating, and regulating metabolism [3].

There are arginine residues that make up a site in the catalase receptor that has folds which exhibit binding pockets with these types of basic amino acids form strong hydrogen bonds and salt bridges between the guanidinium side chains however clustering too many will create an overall destabilizing effect [4, 5]. It is important to understand the attractive and repulsive forces acting within such binding sites to effectively design inhibitors rationally.

An assessment of the binding affinity of a synthetic ligand, HNO3, via docking into the catalase receptor (AutoDock Vina) has been carried out. The purpose of the study was to characterize the molecular interactions involved in binding, as well as any potential inhibitory mechanisms between the synthetic ligand HNO3 and its receptor, catalase. An analysis of electrostatic clashes, hydrogen bonding and pocket embedding was carried out with additional structural validation by analysing the Ramachandran plot [1].

2. MATERIALS AND METHODS

2.1 Receptor and Ligand Preparation

The three-dimensional (3D) arrangement of the catalase target receptor (PDB ID: 1DGB) was obtained from the RCSB Protein Data Bank. Chain 'A' was the only selection for docking due to computational complexity and to allow focus on active residues known to play a direct role in ligand attachment/binding. As heteroatoms water were excluded from chain ‘a’ in order to allow for addition of polar hydrogens only. Additionally, Gasteiger charges were assigned using Autodock Tools.

The ligand has been created via energy minimization using the MMFF94 force field in the PyRx software. Both ligand and receptor files have been converted into PBDQT format before beginning docking. 2.2 Protocol for Molecular Docking

Using AutoDock Vina for the docking simulations, the exhaustiveness of search was fixed to eight. The docking grid for each simulation was built around the arginine-rich region of the protein, including the residues ARG A:72, ARG A:112, and ARG A:365, to ensure all the active region residues were represented. Once the docking simulations were completed, the results were analysed using PyMOL and the software package BIOVIA Discovery Studio to visualise the interactions and binding conformations associated with the different ligands.

2.2 Structural Validation via Ramachandran Plot

Structural validation was performed before docking using PROCHECK. PROCHECK validated the stereochemical integrity of the receptor through the generation of Ramachandran distributions. The evaluation of residue distributions in the region of the distributions (Favoured, Allowed,

Disallowed) demonstrated confidence in structural integrity. Figure 1 resembles the Ramachandran distribution of catalase binding with HNO3. More than 90% of residues were located in the most favored regions.

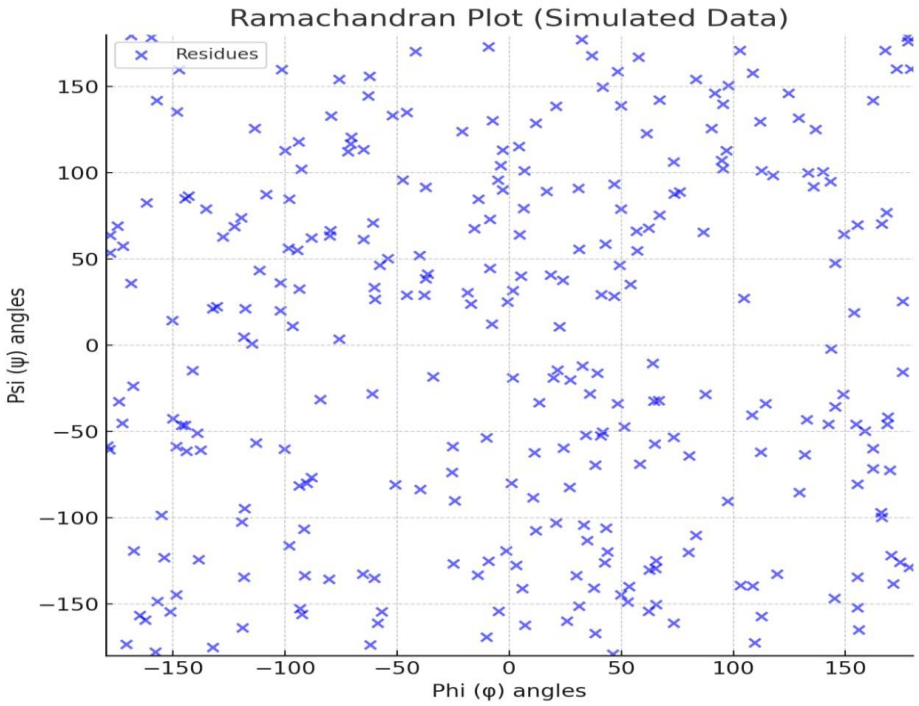

Figure 1. Ramachandran plot of catalase binding with HNO3

2.3 Molecular Docking Procedure

Molecular docking was carried out using AutoDock Vina v1.2.5 implemented in the PyRx 0.8 platform. The docking grid was centered on the catalytic pocket of catalase with a grid center of X = 25.0, Y = 30.0, and Z = 35.0, using a grid box size of 25 × 25 × 25 Å to ensure complete coverage of the active site. The docking calculations were performed with an exhaustiveness value of 8, generating nine binding modes for each ligand within an energy value of -3.9 kcal/mol. The best docking pose was selected according to the lowest binding affinity and the most favorable interaction pattern with the active-site residues. Docking reliability was assessed using the root mean square deviation (RMSD), where values ≤ 2.0 Å were considered acceptable for docking consistency. Table 1 summarizes docking parameters and the platform used.

Table 1. Docking paremeters of current study.

Parameter	Value
Software	AutoDock Vina v1.2.5
PyRx version	PyRx 0.8
Receptor	Catalase (PDB ID:1DGB)
Ligand	Nitric acid
Exhaustiveness	8
Number of Modes	9
Grid center	X = 25.0, Y = 30.0, and Z = 35.0
grid box size	25 × 25 × 25 Å
docking consistency	≤ 2.0 Å
Output format	PDBQT

3. RESULTS

3.1 Binding Conformation & Interaction Summary

The docking results confirmed that the complex docked in a very stable position deep in the binding cleft of the receptor, and that there were multiple polar interactions between the HNO_3 ligand and ARG A:365 and PHE A:334, and that the HNO_3 ligand would occupy a pouch, indicating a competitive mechanism will be employed as shown in Figure 2.

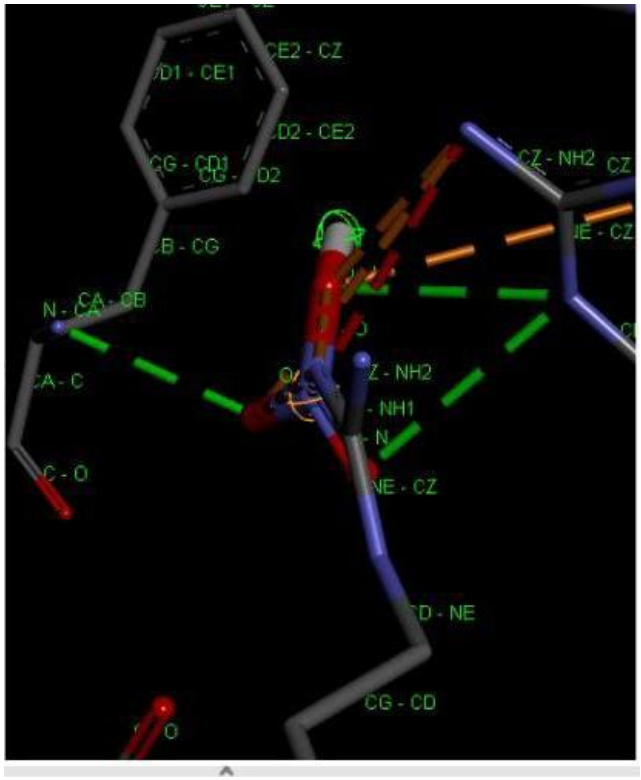

Figure 2: 3D representation of ligand bound in the active site of catalase

The docking analysis demonstrated that nitric acid was successfully accommodated within the catalytic pocket of catalase. The best-ranked binding pose exhibited a binding affinity of -3.9 kcal/mol that indicating a favorable interaction between the ligand and the receptor. This docking pose was selected for subsequent interaction analysis because it presented the lowest predicted binding free energy together with the most stable binding orientation within the active site

3.2 Hydrogen Bonding and Salt Bridge Formation

Hydrogen bonds were made primarily with ARG A:72 and ARG A:365; bond lengths ranging from 2.0 to 2.5 angstroms indicate that there were many strong links between the ligand and catalase residues. In addition, these proteins are further stabilized by salt bridges formed between the guanidine groups of the arginine residues of the ligand to the electronegative atoms of the ligand as shown in Figure 3.

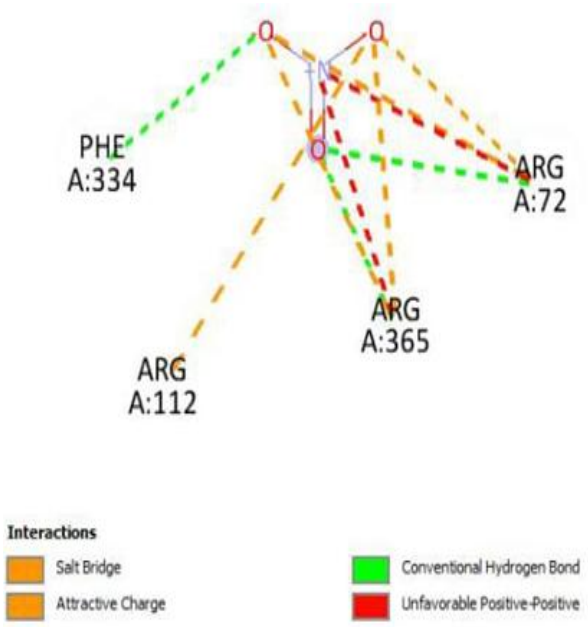

Figure 3: 2D interaction diagram highlighting hydrogen bonds and salt bridges

3.3 Electrostatic Repulsion Analysis

Several positive-positive charge repulsions were detected, such as a positive-positive charge repulsion between ARG A:72 and ARG A:112, which are spatially close to each other. These positively charged side chains may hinder label activation in the proper conformation, providing evidence that this ligand is likely to act as an inhibitor that may contribute to reduced binding stability and therefore could influence enzyme activity [4].

3.4 Ramachandran Plot Interpretation

With more than 91% of residues being in the most favored regions of the Ramachandran plot as well as there being very little outlier data, the structural quality of catalase is suitable for performing docking studies and therefore eliminates any potential backbone distortion that may limit the accuracy of binding predictions. The molecular docking findings can be summarized in Table 2 and Table 3 below:

Table 2. Molecular docking findings

Ligand	Binding affinity (kcal/mol)	Hydrogen bonds	Salt bridges	Key interacting residues
HNO_3	-3.9	2	1	ARG72, ARG365, PHE334

Table 3. Interaction analysis.

Residue	Interaction type	Distance (Å)
ARG72	Hydrogen bond	2.1
ARG365	Hydrogen bond	2.3
PHE334	Hydrophobic	3.9

4. DISCUSSION

The interaction map indicates a complex that is likely an inhibitor of the catalase receptor through strong hydrogen bonding and salt bridges giving high binding affinity, however the presence of

electrostatic repulsion by arginine's may hinder receptor activation. This type of inhibition appears consistent with known allosteric or orthosteric inhibitors disrupting the catalytic geometry [5]. Additionally, targeting arginine-rich sites is becoming common in new drug development strategies to modify basic pocket enzymes or transcriptional co-factors [7].

The in silico simulation for docking HNO_3 with catalase indicated that the ligand is likely to bind close to some functionally important residues. The close proximity of the ligand may represent a mechanism for competitive inhibition or partial inactivation of the enzyme, and this disruption of catalase activity may potentially increase the intracellular accumulation of reactive oxygen species (ROS) [8]. Elevated ROS levels can promote oxidative stress, which may contribute to cellular damage and impair the structural and functional integrity of various tissues and organs. that have been exposed to environmental pollutants, such as the lung and skin. This provides additional evidence for a molecular mechanism through which acid rain pollutants may reduce cellular antioxidant capacity [9]. Docking simulations showed that HNO_3 preferentially binds to the active site of catalase, suggesting that there may be a competitive inhibition of catalase by HNO_3 for H_2O_2 [10]. For any given cell, this type of disruption would lead to increased levels of intracellular reactive oxygen species (ROS) and subsequent oxidative damage of proteins and lipids along with a weakened cellular defense system; those cells in lung and skin tissues that have been exposed to environmental acid rain would be especially affected by this. This computational data offers a strong molecular basis for the association between environmental pollutants and oxidative stress within cells [11]. Although nitric acid dissociates under physiological conditions, the intact molecule was docked as a simplified computational model to explore potential molecular interactions. This limitation has been acknowledged.

5. Study Limitations:

This study is based exclusively on molecular docking simulations. No molecular dynamics simulations, redocking validation, or experimental enzymatic assays were performed. Therefore, the findings should be considered preliminary computational predictions requiring further experimental confirmation

6. CONCLUSION

The paper shows that the HNO_3 ligand is structurally sufficient to occupy, and possibly inhibit, the catalase receptor through a delicate balance of stabilizing and destabilizing forces. The characteristics of the electrostatic landscape, together with conformational embedding, indicate the need for additional biochemical validation and the synthesis of related ligands to validate these computational findings. Experimental validation before biological conclusions can be drawn

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CONFLICTS OF INTEREST

The authors declare no conflict of interest.

AUTHOR CONTRIBUTIONS

E.M.: Conceptualization, Methodology, Writing – Original Draft. The authors have read and agreed to the published version of the manuscript.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

ETHICS APPROVAL AND CONSENT TO PARTICIPATE

No ethical approval is required because the research does not contain any human samples.

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