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Exploring the Interaction of [Pb(II)(Tpy)(NO_3)$_2$] Supramolecular Complex with some Cancer Proteins Via Molecular Docking Studies

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ABSTRACT

This research involved in-depth analysis of the supramolecular complex [Pb(II)(Tpy)(NO_3)$_2$] through a computational technique. The *in silico* molecular docking investigations were conducted to explore the interactions of [Pb(II)(Tpy)(NO_3)$_2$] with selected cancer proteins. Four cancer protein structures were downloaded from the protein databank. These include 1XF0 for prostate cancer, 3QTR for cervical cancer, 4DRH for breast cancer, and 4ATK for melanoma skin cancer. For each protein, the metal complex and the standard anticancer drug were docked as ligands. The molecular docking simulations gave a large negative MolDock score for the Pb(II) complex, the largest being -161.837 kCal/mol for prostate cancer protein. This implies that the complex demonstrates promising anticancer potential, and the strongest inhibition would be against prostate cancer. This research offers valuable insights into the potential of [Pb(II)(Tpy)(NO_3)$_2$] as a promising candidate for targeted cancer therapy.

KEYWORDS: Cancer, protein interactions, molecular docking, Pb(II) complex, supramolecular complex.

INTRODUCTION

Metal-based therapeutics are pharmaceutical chemical compounds in which metal complexes serve as the biologically active component for the diagnosis, treatment, or prevention of diseases. Unlike traditional organic pharmaceutical chemical compounds that are primarily carbon-based, metal-containing drugs possess unique physicochemical properties arising from the presence of metal centers, which includes diverse coordination geometries, variable oxidation states, and redox activity [1-3]. These properties enable metal complexes to interact effectively with biological molecules such as DNA, proteins, and enzymes, thereby influencing important biochemical pathways. The earlier discovery of Cisplatin revolutionized the field of medicinal inorganic chemistry and demonstrated the enormous therapeutic potential of metal complexes in medicine [4]. Cisplatin and its derivatives have been successfully employed in the treatment of several cancers, including ovarian, lung, and testicular cancers, which stimulated further investigations into other biologically active metal complexes [4-5].

Metal-based therapeutics have emerged as promising alternatives to purely organic drugs because they can overcome several associated limitations, including poor selectivity, low bioavailability, and drug resistance. These advantages arise from the incorporation of transition metal ions, which can modulate redox properties, coordination geometry, and lipophilicity of the resulting complexes. Such modifications significantly influence the pharmacokinetic behavior and mechanisms of action of the therapeutic agents, thereby enhancing their biological activity and therapeutic efficacy [6-7]. One of the major advantages of metal-based therapeutics is their structural versatility, which allows the formation of complexes with tailored biological activities and improved selectivity toward disease targets. Metal ions can coordinate with a wide range of ligands, thereby modifying the pharmacological, electronic, and steric properties of the resulting complexes. In addition, metal complexes often exhibit mechanisms of action that differ from those of conventional organic drugs, making them useful in overcoming drug resistance. Their ability to participate in redox reactions and catalytic biological processes also contributes to enhanced antimicrobial, anticancer, anti-inflammatory, and diagnostic applications [8]. Furthermore, the incorporation of bioactive ligands into metal complexes may improve drug solubility, stability, and bioavailability while reducing toxicity. Owing to these unique properties, metal-based therapeutics continue to attract significant attention in medicinal chemistry and coordination chemistry research as promising alternatives for the development of next-generation drugs [8-11].

The known toxicity of lead has traditionally limited its therapeutic use. Some recent studies suggest that complexation with ligands can mitigate this drawback. Studies on the interaction of Pb^{2+} ions with various organic compounds have shown that complex formation can significantly modify the chemical behavior, reactivity, and mobility of lead in solution. Through coordination, Pb^{2+} is effectively bound within stable metal–ligand frameworks, thereby reducing the concentration of free, bioavailable toxic ions in the system. This complexation process plays a crucial role in decreasing the immediate reactivity and toxicity associated with uncoordinated Pb^{2+} species. It is well established that free Pb^{2+} ions are highly toxic; however, coordination with suitable ligands such as terpyridine and Schiff base derivatives can substantially alter their biological impact. Such ligand binding reduces the bioavailability of Pb^{2+} as a toxic species, stabilizes the metal center through chelation, and limits its uncontrolled interaction with biological targets. In addition, metal complexation has been associated with the emergence of enhanced or modified biological properties, including antioxidant, antimicrobial, and anticancer activities, which are typically absent in the free metal ion [12-15].

Researchers have reported that Pb(II) complexes containing carbothioamide ligands exhibited enhanced biological activities, particularly antimicrobial effects, when compared with the corresponding free ligands [16]. Tella et al. [17] synthesized and characterized a Zn(II) complex of amoxicillin and further investigated its interaction properties. Similarly, Olawale et al. [16] synthesized a copper–pyrazinamide complex containing an anti-tuberculous drug, where the bioactivity against *Mycobacterium* tuberculosis was theoretically evaluated alongside toxicity studies on rat liver models. In another study, some researchers investigated the antimicrobial activity of a synthesized Zn(II) complex of meso-tetraphenylporphyrin [18]. Furthermore, a group of researchers reported the synthesis and structural characterization of Pb(II) and related transition metal complexes derived from a thiosemicarbazone Schiff base ligand. Spectroscopic analyses confirmed successful coordination between the ligand and metal ions, while biological studies demonstrated that the Pb(II) complex exhibited significant antibacterial activity against both Gram-positive and Gram-negative bacteria. The improved biological activity was attributed to metal coordination, which possibly enhanced the lipophilicity of the complexes and facilitated stronger interactions with microbial cell components [19].

Olawale et al [20] presented the synthesis, characterization, and computational investigation of the supramolecular complex $[Pb(Tpy)(NO_3)_2]$ using Density Functional Theory (DFT), ADME prediction, and molecular docking studies. The DFT calculations revealed band gap and global hardness values of 1.06 and 0.53 eV, respectively, indicating high chemical reactivity and potential applicability in conductivity-related studies. Furthermore, molecular docking against the serotonin 5-HTR2A receptor showed a binding affinity comparable to that of risperidone, suggesting that the Pb(II) complex could serve as a promising candidate for targeted psychotic therapy. Owing to the growing pharmacological relevance of Pb(II) metal complexes, the present study explores the interaction of the supramolecular complex [Pb(II)(Tpy)(NO_3)$_2$] with some cancer-related proteins using *in silico* molecular docking studies.

MATERIALS AND METHODS

Materials and Physical Measurements

Molecular Docking Methodology

The molecular docking simulation was carried out using Molegro Virtual Docker program [21] installed on a PC with Windows 10 Pro Operating System. The optimized structures of the Pb(II) complex and doxorubicin; a standard anticancer drug retrieved from PubChem database (https://pubchem.ncbi.nlm.nih.gov/#query=doxorubicin) were stored in pdb format. Then, they were converted to Mol file format, an acceptable Molegro format for ligands, using Open Babel GUI program.

Four cancer protein structures were downloaded from the protein databank (https://www.rcsb.org/). These include the following PDB IDs: 1XF0 for prostate cancer, 3QTR for cervical cancer, 4DRH for breast cancer, and 4ATK for melanoma skin cancer. For each protein, the metal complex and the standard anticancer drug were docked as ligands. First, each protein was uploaded to the workspace in Molegro program. A surface was created for the protein, and the cavities detected. The cavity defines the binding pocket where the co-crystalline ligand sits. It is also referred to as the binding site. Thereafter, active co-crystalline ligand of the protein was removed.

Then, the Mol files of the ligands (metal complex and standard drug) were uploaded to the workspace and prepared using the Molegro preparation engine. The docking simulation was carried out with an energy minimization of the molecules, enabling energy thresholds at the defined parameters of the binding pocket. The parameters include a uniform grid resolution of 0.3 Å and radius of 15. Also, the respective binding site center X, Y, and Z of 18.66, 39.33 and 3.46 for 1XF0; 93.55, 69.30 and -49.50 for 3QTR; 8.40, 18.91 and 6.43 for 4DRH; and 36.89, 8.57 and 7.53 for 4 ATK.

RESULTS AND DISCUSSION

Molecular Docking Simulation Analysis

Molecular docking is an effective *in silico* approach used to investigate ligand–receptor interactions by predicting the binding behavior and orientation of small molecules (ligands) within the active site of target proteins (receptors) [22-24]. Sharma and Bharti [25] reported that a Pb(II) complex of a novel ligand, formed from a mixture of salicyaldehyde and phenylhydrazine, demonstrated good antioxidant activity. Furthermore, the anticancer effect of certain trihydroxyflavones have been related to their antioxidant activity [25]. Here, the [Pb(II)(Tpy)(NO_3)$_2$] complex and the standard drug are treated as ligands and docked against four cancer proteins. The results of the molecular docking simulations are presented in Table 1.

Table 1: Molecular Docking Scores

	MolDock score (kcal/mol)	Rerank score (kcal/mol)	HBond energy (kcal/mol)	Interaction energy (kcal/mol)	Torsion	Hydrogen bonding residues
1xf0-dox	-62.829	130.581	-3.88127	-130.389	5	Ser118, Tyr317, Tyr24, Ser310
1xf0-Pb(II)	-161.837	-116.924	-1.03984	-167.093	7	Try216, Tyr319, Asn167
3qtr-dox	-119.914	-107.479	-13.3959	-188.04	5	Asp145
3qtr-Pb(II)	-149.075	-101.035	-4.10423	-144.98	7	Asp145, Ile110, Lys89, Asp86
4drh-dox	-75.537	2.38903	-5.19885	-124.349	5	Phe2048, Cys2085, Gln2082
4drh-Pb(II)	-126.090	-96.8298	-12.1956	-134.159	7	Arg2086, Gln2082
4atk-dox	-53.645	-67.725	-0.687751	-107.966	5	Arg223
4atk-Pb(II)	-90.932	-60.775	0	-89.8494	7	-

The inhibitory activity of molecules is associated with the molecular docking (MolDock) scores. A positive MolDock score suggests poor inhibitory activity, small negative MolDock score suggests moderate inhibitory activity and large negative MolDock score implies very strong inhibitory activity [26]. Generally, both the complex and doxorubicin showed excellent inhibitory activities against all four cancer proteins. Interestingly, the Pb(II) complex demonstrated stronger inhibitory activity than the standard drug for all four cancer proteins. This suggests that metal complex could make a promising anticancer drug candidate with possible higher activity than doxorubicin. While doxorubicin showed the strongest inhibitory activity against cervical cancer, the Pb(II) complex showed strongest inhibitory activity against prostate cancer.

Rerank scoring from the simulation shed more light on the stability of the biological complex. Reranking score is a metric obtained by applying a secondary, computationally intensive scoring function to the top ligand poses produced by an initial, faster docking algorithm. It is designed to filter out false positives and improve the accuracy of predicted binding affinities [27,28]. As seen in table 1, the Pb(II) complex shows much higher stability and inhibition potential against both prostate and breast cancers, than doxorubicin. On the other hand, the Pb(II) complex has reduced stability and inhibition potential against cervical and melanoma skin cancers, than doxorubicin.

The hydrogen bond energy is a crucial electrostatic component of the overall binding affinity, primary calculated using distance and angle constraints within the docking program's scoring function [29]. Generally, as shown in table 1, doxorubicin has lower (more negative) hydrogen bond energy than the Pb(II) complex, for all the protein complexes. This is also reflected in the number of hydrogen bonding residues. Notably, 4ATK-Pb(II) complex has zero hydrogen bond energy value, shown by no hydrogen bonding residue. The general trend of the hydrogen bonding in both biological complexes can be attributed to the presence of more oxo and hydroxyl groups in doxorubicin, which can form relevant hydrogen bonding some amino acids in the target protein.

The interaction energy is the direct non-bonded energetic sum between a ligand and a target protein in a specific docked pose [29-31]. For each pose with zero RMSD whose binding pose was selected for analysis, their interaction energies are presented in Table 1. Here, the interaction energies for doxorubicin and the Pb(II) complexes have trend like the re-rank scores. In summary, the number torsions (dihedral angles) for doxorubicin and the Pb(II) are 5 and 7, respectively.

A solid ribbon display of the biological (protein-ligand) complexes containing the cancer proteins and docked ligands are presented in Figure 1.

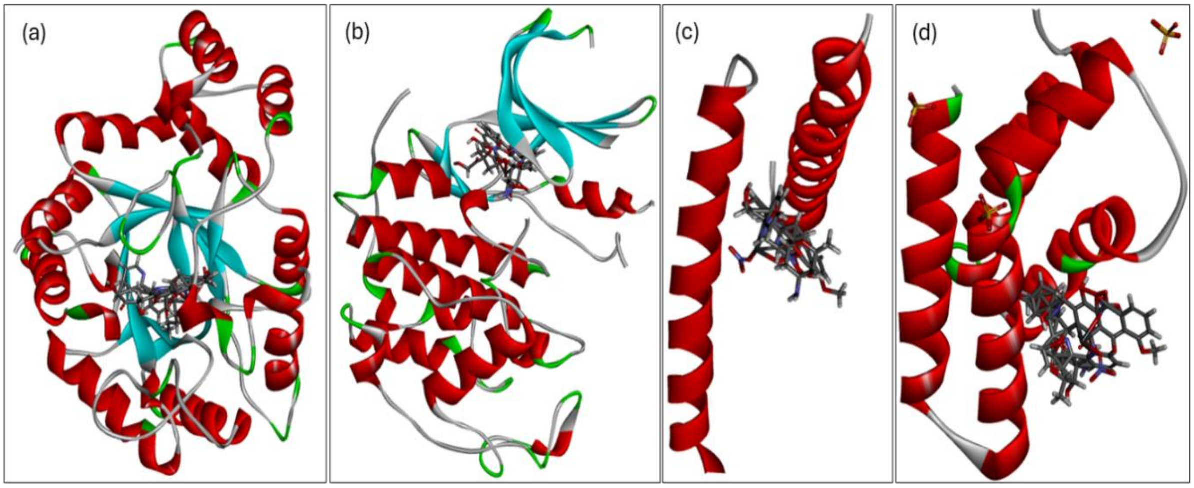

Figure 1: Solid ribbon display of the biological complexes showing both ligands docked unto the active sites of (a) 1XF0 (b) 3QTR (c) 4ATK (d) 4DRH.

2-dimensional diagrams showing the interactions between both ligands and each of the four cancer proteins are presented in Figures 2-5. Generally, all the biological complexes are stabilized by van der Waals, conventional hydrogen bond and pi-alkyl interactions. Also, all the complexes except 1XF0-Pb(II) and 4DRH-Pb(II) complexes, are stabilized by carbon hydrogen bond interaction. 1XF0-Doxorubicin complex (Figure 2a) is stabilized by unfavourable bump interactions to Ser308, Trp86, Ser118, and Tyr317 residues; pi-cation interaction to Trp86 residue; pi-anion interactions to His117 residue; and pi-pi stacked interactions to Trp227 and Phe306 residues. The 1XF0-Pb(II) complex (Figure 2b) is stabilized by attractive charge to Phe306, pi-cation interaction to Phe311; pi-anion interaction to Glu192; pi-sigma interaction to Phe306 residue.

3QTR-Doxorubicin complex (Figure 3a) is stabilized, in addition to stated common interactions, by attractive charge interaction three Lysine (Lys33, Lys89 and Lys129) residues; unfavourable interaction to Gln131 residue; and pi-pi stacked interaction to Phe82 residue. 3QTR-Pb(II) complex (Figure 3b) is stabilized by attractive charge interaction to Lys33 and Asp145 residues; pi-cation interaction to both Asp86 and Asp145 residues; pi-anion interactions to Lys89 and Lys129 residues; and pi-pi stacked interactions one each from the two aromatic ring to Phe80 and Phe82 residues.

4ATK-Doxorubicin complex (Figure 4a) is stabilized by pi-anion and pi-cation interactions to Glu226 and Arg223 residues; and pi-sigma interaction from an aromatic ring to Arg223 residue. The 4ATK-Pb(II) complex (Figure 4b) is stabilized by a salt bridge, attractive charge, unfavourable positive-positive and amide-pi stacked interactions, all connected Arg223 residue. These suggest that Arg223 amino acid residue is a key residue in the inhibition of melanoma skin cancer.

4DRH-Doxorubicin complex (Figure 5a) is stabilized by unfavourable bump and unfavourable negative-negative interactions to Gln2082 and Glu2052, respectively. Others include attractive charge, pi-cation, and pi-anion interactions to Glu2052 and Arg2086 residues. 4DRH-Pb(II) complex (Figure 5b) is stabilized by attractive charge and pi-anion interactions to Arg2086 and Glu2052 residues, respectively. Others include unfavourable positive-positive, unfavourable negative-negative and unfavourable donor-donor interactions to Gln2082, Glu2052 and Arg2086 residues, respectively.

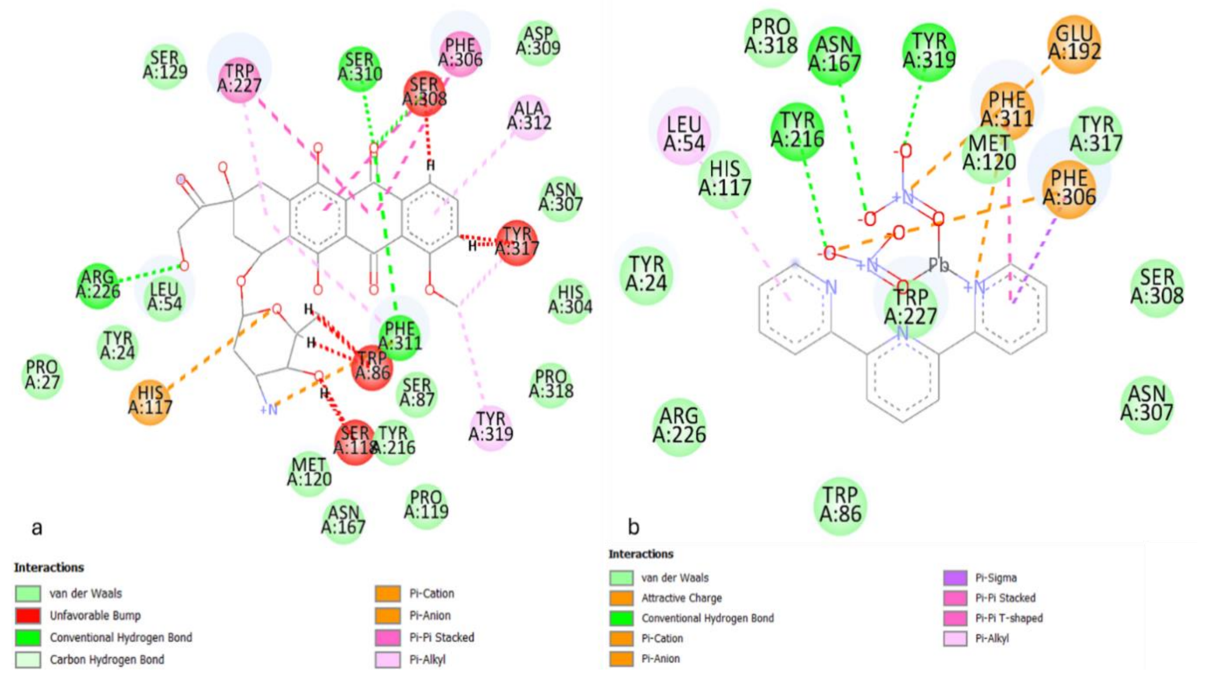

Figure 2: 2-dimensional diagrams of the interactions involving (a) Doxorubicin, (b) Pb, and prostate cancer (PDB ID: 1XF0) protein.

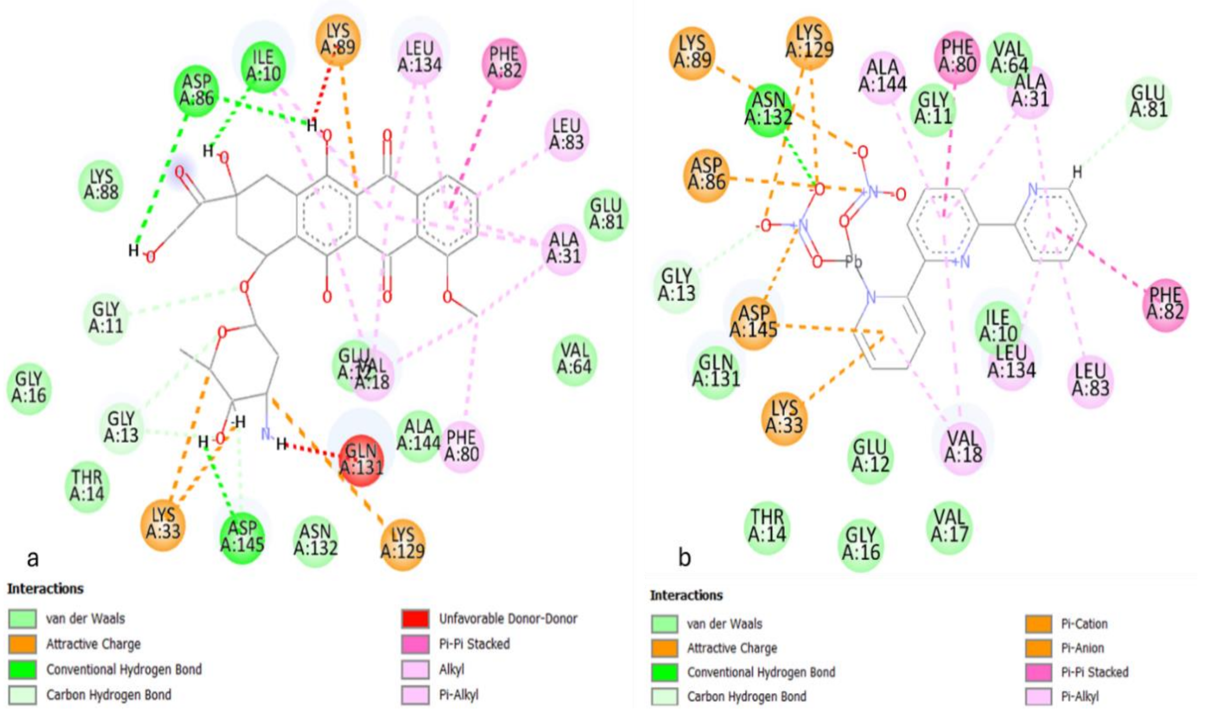

Figure 3: 2-dimensional diagrams of the interactions involving (a) Doxorubicin, (b) Pb, and cervical cancer (PDB ID: 3QTR) protein.

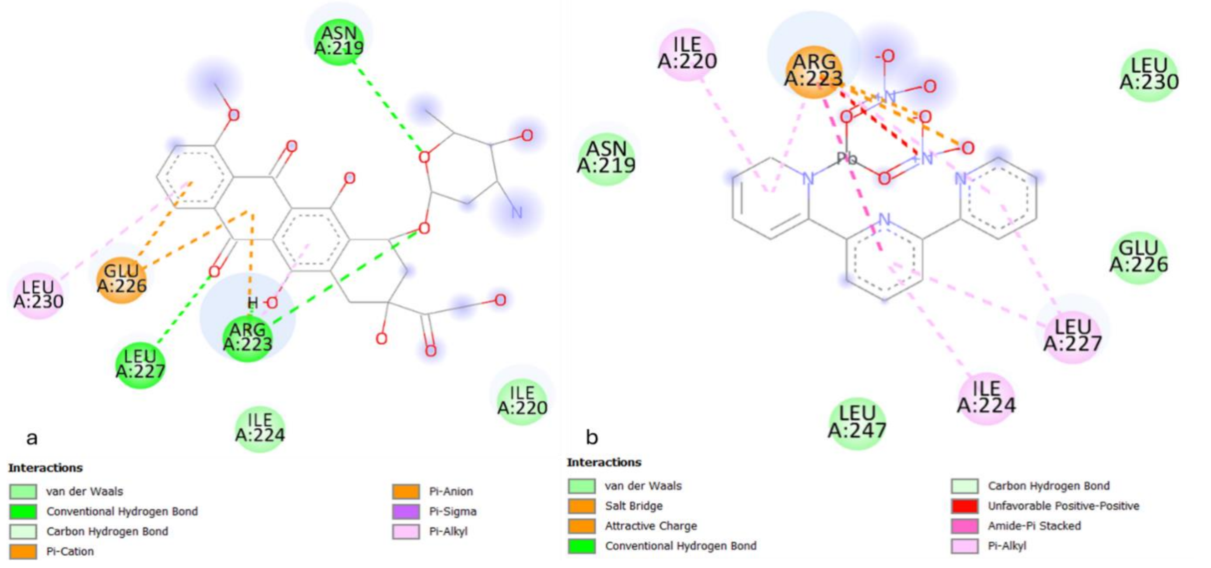

Figure 4: 2-dimensional diagrams of the interactions involving (a) Doxorubicin, (b) Pb, and melanoma skin cancer (PDB ID: 4ATK) protein.

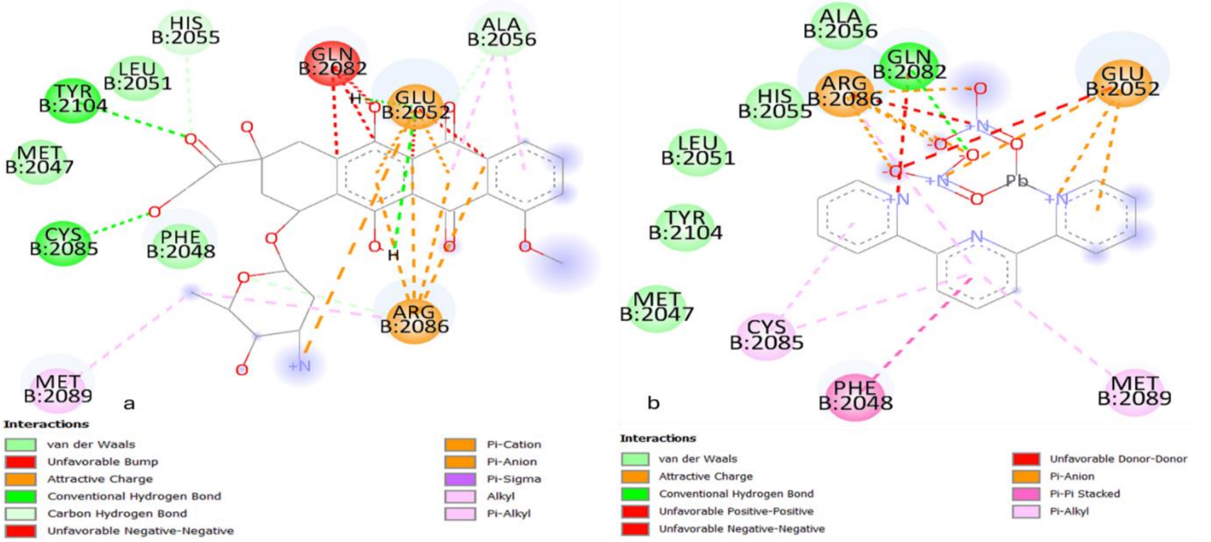

Figure 5: 2-dimensional diagrams of the interactions involving (a) Doxorubicin, (b) Pb, and breast cancer (PDB ID: 4DRH) protein.

The physicochemical analysis of the Pb(II) complex, as reported in our recent article [20], informs that the molecule obeys the Verber's rule (rotatable bond ≤ 10; polar surface area ≤ 140 $Å^2$), indicating a good oral bioavailability. Meanwhile, it obeys the Lipinski's rule of 5 partially with 2 violations. This suggests poor drug likeness but a structural modification could improve its features.

CONCLUSION

The comprehensive exploration of the supramolecular complex [Pb(II)(Tpy)(NO_3)$_2$] in this study reveals its probable potential for advancing cancer research and therapy. Through sophisticated computational analyses involving molecular docking simulations, this research offers valuable insights into the molecular interactions of the complex with cancer proteins. The study demonstrates the potential of [Pb(II)(Tpy)(NO_3)$_2$] as a promising candidate for targeted cancer therapy. Additionally, *in silico* molecular docking simulations indicate superior anticancer potential for the complex compared to the established drug doxorubicin. This investigation enhances an understanding of the Pb(II) complex's molecular behavior, providing critical insights for targeted drug design. Further exploration of [Pb(II)(Tpy)(NO_3)$_2$] in cancer treatment represents a promising avenue for advancing precision medicine and elevating therapeutic outcomes in oncology.

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