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Evaluating *Andrographis Paniculata* Phytochemicals as Potentisal Glioma Therapeutics via Molecular Docking Approach

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Abstract

Glioneuronal tumors and gliomas are grade I tumors classified by the World Health Organization (WHO). They typically grow slowly and primarily affect infants, children, and teenagers, but can also occur in adults. They mostly cause seizures caused by gangliomas. Most current treatments include surgery and radiotherapy. Since this disease affects children, the current treatments may cause complications. Andrographis paniculata is a medicinal plant that is native to the Indian subcontinent, some parts of China, and Southeast Asia. It has lance-shaped leaves with white flowers with purple streaks. It has short, upright, and branching stems. It has been extensively used in Indian and Chinese traditional medicine. It has anti-inflammatory, antibacterial, hepatoprotective, anti-tumor, and immunomodulatory qualities. Its phytocompounds can suppress the growth of tumor cells. In this study, I explore using Andrographis paniculata phytocompounds against Glioneuronal and glioma tumors. This study explores the in situ and molecular docking analysis. The in-situ analysis was done by SwissADME. The molecular docking was done using the PyRx tool using Autodock Vina software. The Anti-apoptotic protein (Bcl-xl) inhibits programmed cell death. Similarly, Phosphoinositide 3-Kinase (PI3K) is an important signalling pathway that is dysregulated in the case of a tumor. These two proteins were docked against the Andrographis paniculata phytocompounds. The phytocompounds 5-Hydroxy-7,8-dimethoxyflavone, Andrographin, Myristic acid, and Carvacrol showed excellent binding affinity to Bcl-xl and PI3K. Then the protein-phytocompound complex was visualized in Biovia DS software. This study can be further continued by performing molecular dynamics analysis and further in vitro analysis to further understand the therapeutic effect of Andrographis paniculata against Glioneuronal and Gliomas tumors.

Keywords: Glioneuronal tumor, Gliomas, in-silico analysis, molecular docking, Andrographis paniculata, ADME analysis, PI3K and Bcl-xL

INTRODUCTION

Glioneuronal tumors (GNTs) are rare neoplasms of the central nervous system, also called glioneuroid tumors. They are slow-growing tumors that primarily affect newborns, children, and young adults. Although they sometimes occur in adults as well. They frequently have a high correlation with seizures as a symptom, which is a defining clinical characteristic [1]. Glioneuronal tumors (GNTs) are classified as grade I tumors by the World Health Organization (WHO). The WHO categorizes the GNTs between diffuse and non-diffuse forms of gliomas. Glioblastomas, oligodendrogliomas, and astrocytomas are examples of diffuse gliomas. Ependymoma, pleomorphic xanthoastrocytoma, and pilocytic astrocytoma are examples of non-diffuse gliomas [2]. In 2021, the WHO classification identified three main families, which combine histology and molecular genetics.

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Glioneuronal and neuronal include a number of recently identified entities, such as MVNT (multinodular and vacuolating neuronal tumor, associated with MAP2K1 (mitogen-activated protein kinase) and BRAF mutations), DGONC (diffuse glioneuronal tumor with oligodendroglioma-like features and nuclear clusters), MGT (myxoid glioneuronal tumor, linked to PDGFRA (platelet-derived growth factor receptor alpha) mutations), and PLNTY (polymorphous low-grade neuroepithelial tumor of the young, associated with FGFR2 (fibroblast growth factor receptor 2) fusions) [3].The symptoms differ depending on the subtype of gliomas and glioneuronal tumors. The symptoms include drug-resistant seizures, panic episodes, focal epilepsy, increased intracerebral pressure, hydrocephalus, and neurological impairments [4]. Currently, multimodal treatments are used to treat gliomas. It is based on the molecular profile and tumor grade. The treatment mostly entails safe surgical resections, which enhance seizure control and survival for low-level gliomas. The main treatments include surgery, radiotherapy, and temozolomide chemotherapy for high-grade tumors [5]. Most of the treatment for gliomas/glioneuronal tumors requires either surgery or chemotherapy, which may cause multiple complications and side effects, as most patients are young. Thus, finding a drug-like phytocompound against the tumor can be helpful in combating these complications and side effects, improving the current treatments. *Andrographis paniculata*, known as the "king of bitters," is an annual medicinal plant that is indigenous to tropical and subtropical regions of South Asia and Southeast Asia. It is a plant that has lance-shaped leaves and white flowers with purple streaks. It also has short, upright, and branching stems. It is commonly used in Ayurvedic and Chinese medicine. It has anti-inflammatory, antibacterial, anti-tumor, hepatoprotective, and immunomodulatory qualities [6]. *Andrographis paniculata* has strong anti-tumor and anti-cancer properties by increasing TNF-α (tumor necrosis factor-alpha) and natural killer cell activity by preventing angiogenesis through VEGF reduction, stopping the advancement of malignant cell cycles, and triggering death through caspase and mitochondrial pathways [7]. Preclinical research demonstrates that *Andrographis paniculata* subdues the growth of tumor G0/G1 cell cycle arrest (gap 0/gap 1 phase arrest), which is mediated by downregulating CDK4 (cyclin-dependent kinase 4) and upregulating p27 (cyclin-dependent kinase inhibitor p27^Kip1). By boosting lymphocyte proliferation, cytokine production such as IL-2 (interleukin-2) and TNF-α (tumor necrosis factor-alpha), and NK cell (natural killer cell) cytotoxicity, it also induces apoptosis and has immunomodulatory effects [8, 9]. Although *Andrographis paniculata* seems to show excellent anti-tumor properties, there are not many studies on its effect on gliomas/glioneuronal tumors. Given the limitations of conventional therapies, plant-derived bioactive compounds offer a promising alternative Bcl-xL, an anti-apoptotic protein, promotes glioblastoma cell migration, invasion, and stemness; its inhibition reduces tumor aggressiveness [10]. PI3K pathway activation, often due to PIK3CA mutations and PTEN loss, drives uncontrolled tumor growth and survival [11]. This study aims to evaluate the potential of *Andrographis paniculata* phytochemicals to inhibit Bcl-xL and PI3K proteins in gliomas and glioneuronal tumors using silico molecular docking.

METHODOLOGY

Retrieval of Ligands

The IMPPAT (Indian Medicinal Plants, Phytochemistry, and Therapeutics) database (https://cb.imsc.res.in/imppat/) was used to find bioactive ligands. IMPPAT serves as a curated resource that gathers data on over 1,700 Indian medicinal plants, their more than 10,000 phytochemicals, and their related therapeutic applications [12]. A total of 77 possible phytocompounds of *Andrographis paniculata* were retrieved. The ligand structures were retrieved from PubChem (https://pubchem.ncbi.nlm.nih.gov/) in SDF format [13].

Retrieval of Proteins

The crystal structure of Bcl-xL with PDB ID 4QVF was downloaded from the RCSB-PDB database (https://www.rcsb.org/structure/4QVF), and that of PI3K with PDB ID 4OVV was downloaded from the RCSB-PDB database (https://www.rcsb.org/structure/4OVV). The proteins were downloaded in the legacy PDB format [14]. The protein structure was validated by generating the Ramchandran plot of both proteins using the PDBSUM tool generated (https://www.ebi.ac.uk/thornton-srv/databases/pdbsum) [15].

In Silico Pharmacology Studies of *Andrographis Paniculata* Compounds

The molecular structure of the phytocompounds was retrieved to evaluate the pharmacological properties, which was done using SwissADME (http://www.swissadme.ch) [16]. The pharmacological properties evaluated are GI absorption, bioavailability, blood-brain barrier pains, and brenk. The best ligands are then chosen using the LIPINSKI rule of five. ProTox 3.0(https://tox.charite.de/protox3/) was employed to evaluate the toxicity of the ligands [17].

Protein Purification

Proteins were initially prepared for docking by adhering to a standard purification procedure. Given that the crystallographic structure may not accurately represent the free energy of water molecules, all crystallographic waters were eliminated to prevent them from affecting the docking scores. Likewise, any ligands that were pre-bound in the crystal structures were removed to facilitate accurate binding of the chosen ligands. To streamline the models, only chain A was retained while the other chains were discarded. Additionally, polar hydrogen atoms were introduced to enhance the optimization of the protein structure. All steps related to protein preparation were executed using DS Biovia Discovery Studio [18].

Molecular Docking

The purified proteins (Bcl-xL and PI3K) were loaded as a macromolecule, and the *Andrographis paniculata* phytocompounds were loaded as ligands into PyRx [19]. The ligands were converted from .SDF format to .PDB format using OPENBABEL [20]. Grid dimensions of center X=119.8466, center Y=-25.6426, and center Z=8.393(Bcl-xl) and of center X=72.8466, center Y=37.7576, and center Z=88.5929(PI3K) were chosen as the active site. The ligands were independently docked against Bcl-xL and PI3K using the Vina software in the PyRx tool, and energy minimization was done [21]. The most effective compounds, 5-Hydroxy-7,8-dimethoxyflavone, Andrographin, Myristic acid, and Carvacrol, were chosen for further research based on their binding affinity with the target protein after the docking findings were received.

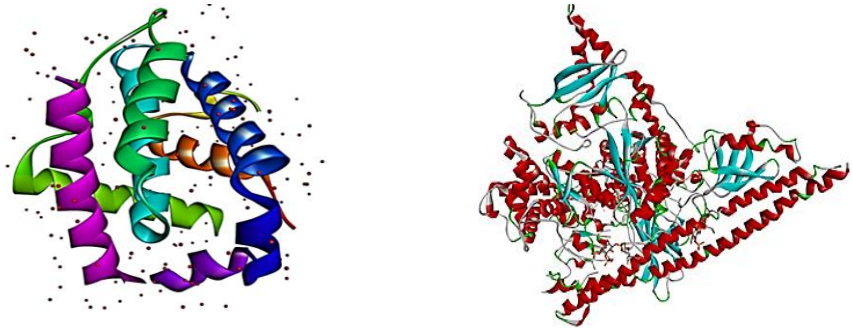
Visualization

The 2D and 3D models were created by downloading the conformations with the best binding scores.PDB format using Dassault Systems BIOVIA Discovery Studio Visualizer [18].

RESULTS

Protein Retrieval

Bcl-xL has a total of 141 amino acid residues. It has two main chains: chain A and chain B. It also has hetero atoms and water molecules. PI3K has a total of 241 amino acid residues. It consists of chain A, chain B, hetero atoms, water, and ligand groups. The protein structure of Bcl-xL and PI3K is shown in Figure 1.



(a) (b)

Figure 1. The retrieved protein structure, a. Bcl-xL and b. PI3K.

Phytocompound Retrieval

A total of 77 phytocompounds were retrieved from the IMPPAT database. The PubChem ID of the phytocompounds was also retrieved. The structure of the phytocompounds was also retrieved in the SMILES format.

Pharmacological Properties

The analysis of drug similarity employs the bioavailability score to evaluate the effectiveness of potential medications intended for oral use. The criteria for this score are based on the structural characteristics of small molecules. The blood brain barrier permeability is an important as.

The Lipinski rule of five is employed to filter small compounds and assess their similarity to drugs. (Table 1). The PAINS score illustrates the medicinal chemistry characteristics of therapeutic compounds by emphasizing substructures in studies that show significant responses regardless of the protein target (Table 2).

For the pharmacologic evaluation, the ligands are screened based on the following parameters: GI absorption(high), Blood-Brain Barrier permeant(yes), bioavailability (>=0.55) and toxicity (>=4). The top four ligands fulfilled all the pharmacological screening parameters.

Table 1. Data for the properties of the Lipinski rule obtained using Swiss absorption, distribution, metabolism, excretion.

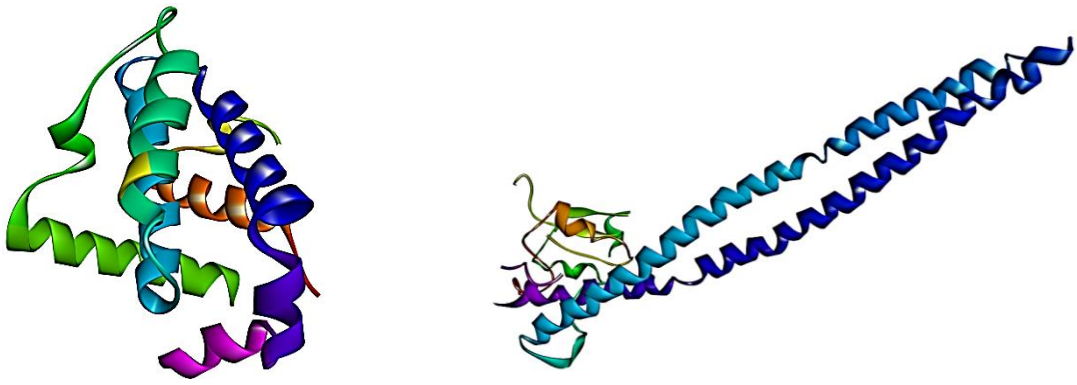
Ligand	Molecular Weight	Mlogp	Hydrogen donors	Hydrogen acceptors	Molar refractivity
5-Hydroxy-7,8-dimethoxyflavone	298.29	1.01	1	5	82.93
Andrographin	328.32	0.7	1	6	89.42
Myristic acid	228.37	3.69	1	2	71.18
Carvacrol	150.22	2.76	1	1	48.01

Table 2. pharmacological properties of the ligand molecules.

Ligand	GI Absorption	BBB Permeant	Bioavailability	Toxicity Class
5-Hydroxy-7,8-dimethoxyflavone	High	Yes	0.55	5
Andrographin	High	Yes	0.55	5
Myristic acid	High	Yes	0.85	4
Carvacrol	High	yes	0.55	4

Protein Purification and Structural Analysis Using RCPlot

The proteins were purified by eliminating heteroatoms and water molecules. In the case of Bcl-xL, chain B was removed, while for PI3K, chain A was deleted. The resulting purified protein structures are shown in Figure 2.



(a) (b)

Figure 2. The purified protein structure of, a. Bcl-xL and b. PI3K.

The energetically acceptable regions where amino acid torsions are oriented against one another in a protein structure are visualized using the Ramachandran map. The Anti-apoptotic Protein and

Phosphoinositide 3-Kinase α (Bcl-xl and PI3K) Ramchandran plot is displayed in Figures 3 and 4, which were created using the PDBSUM-generate tool. The areas highlighted in red on the graph represent the sterically allowed regions that support stable peptide conformations. For computational studies, amino acids need to be predominantly located within the sterically permissible zone, meeting a threshold of over 88%.

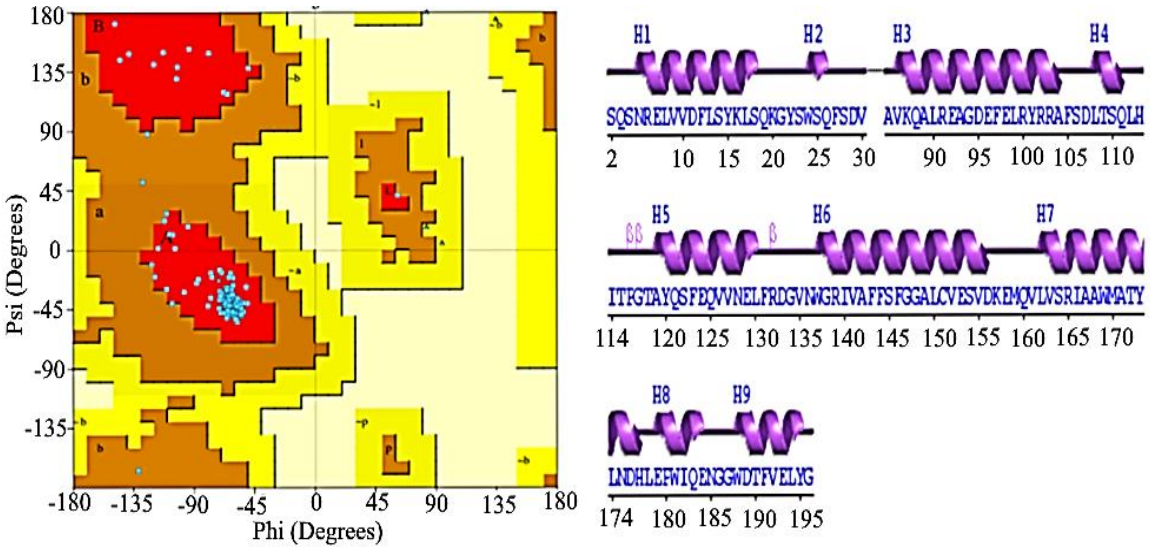


Figure 3. Ramachandran plot of Bcl-xl protein using PDBsum and Secondary structure of protein Bcl-xl.

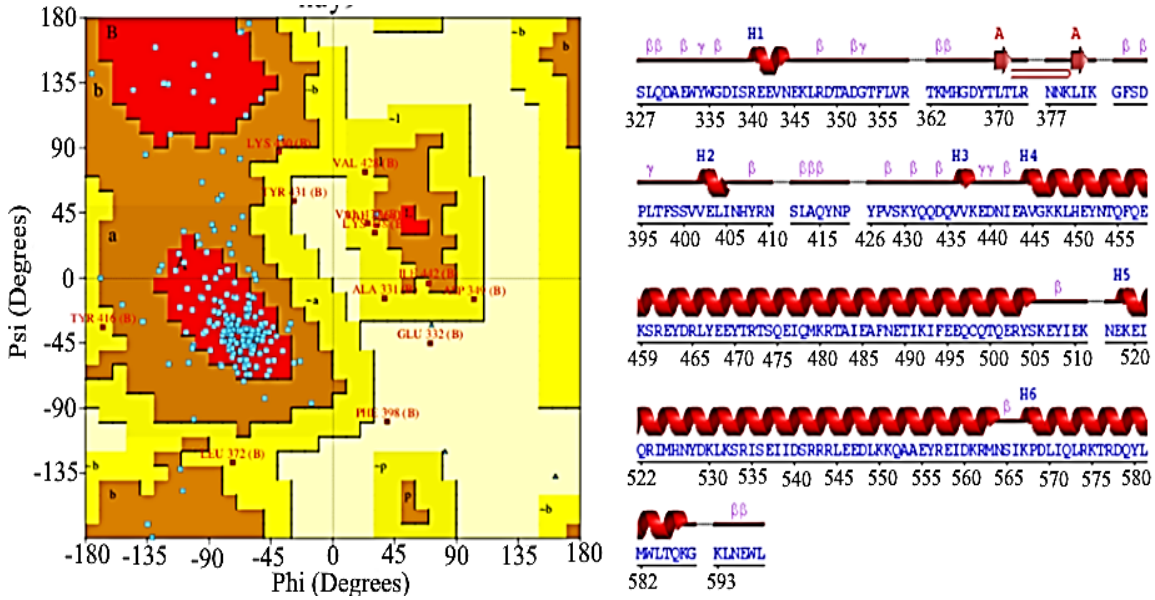


Figure 4. Ramachandran plot of PI3K protein using PDBsum and Secondary structure of protein PI3K.

For Bcl-xL, the approved section contains 93.7%, or 118 residues, of the amino acid residues, whereas the banned region has 0.0% or 0 residue. 10 glycine residues, 2 proline residues, and 126 non-proline and non-glycine residues make up the 141 total residues. The protein Bcl-xl predicted secondary structure includes nine helices, seventeen helix-helix interactions, and three beta turns.

For PI3K, the approved section contains 92%, or 205 residues, of the amino acid residues, whereas the banned region has 1.4% or 3 residues. 10 other regions, 13 end residues,6 glycine residues, 4 proline residues, and 218 non-proline and non-glycine residues make up the 241 total residues. The protein

PI3K predicted secondary structure includes one sheet, one beta hairpin, six helices, three helix-helix interactions, twenty-two beta turns, and seven gamma turns.

Molecular Docking

The ligands 5-Hydroxy-7,8-dimethoxyflavone, Andrographin, Myristic acid and Carvacrol demonstrated the best binding with the target proteins Bcl-xl and PI3K (Tables 3 and 4).

Table 3. Binding affinity of the ligands with proteins Bcl-xl.

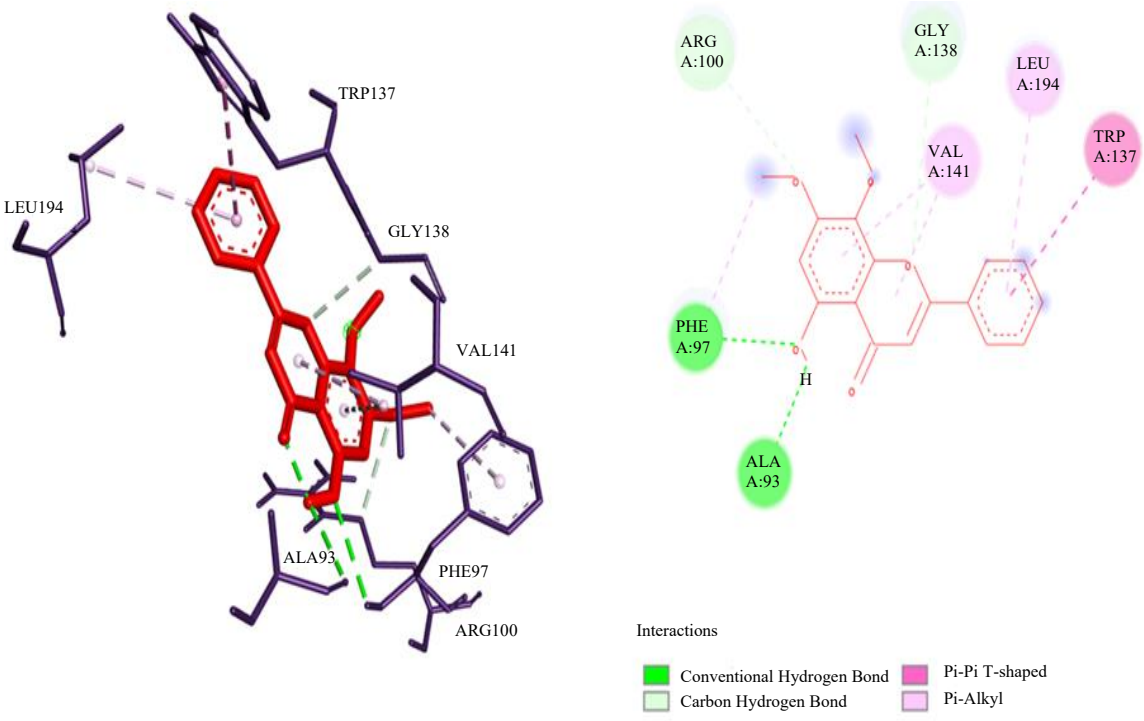
Ligands	Binding affinity of Bcl-xl(kcal/mol)
Andrographin	-7
5-Hydroxy-7,8-dimethoxyflavone	-6.6
Myristic acid	-5.2
Carvacrol	-5.9

Table 4. Binding affinity of the ligands with proteins PI3K.

Ligands	Binding affinity of PI3K
5-Hydroxy-7,8-dimethoxyflavone	-7.7
Andrographin	-6.9
Myristic acid	-4.7
Carvacrol	-6.3

Visualization

The ligand Andrographin has the best binding affinity to the protein Bcl-xl and the ligand 5-Hydroxy-7,8-dimethoxyflavone has the best binding affinity to the protein PI3K, the docked complex was visualized in biovia. From the 3D and 2D interaction diagram (Figures 5 and 6), it is evident that the ligand is bound to the amino groups including LYS 20, GLN 19, ASP 95, ARG 102, GLU 98, LYS 16, ALA 149, And VAL 152 for Bcl-xl AND VAL 401, LEU 396, PHE 398, TRY 368, VAL 357, LEU 404 AND LYS 382 for PI3K.



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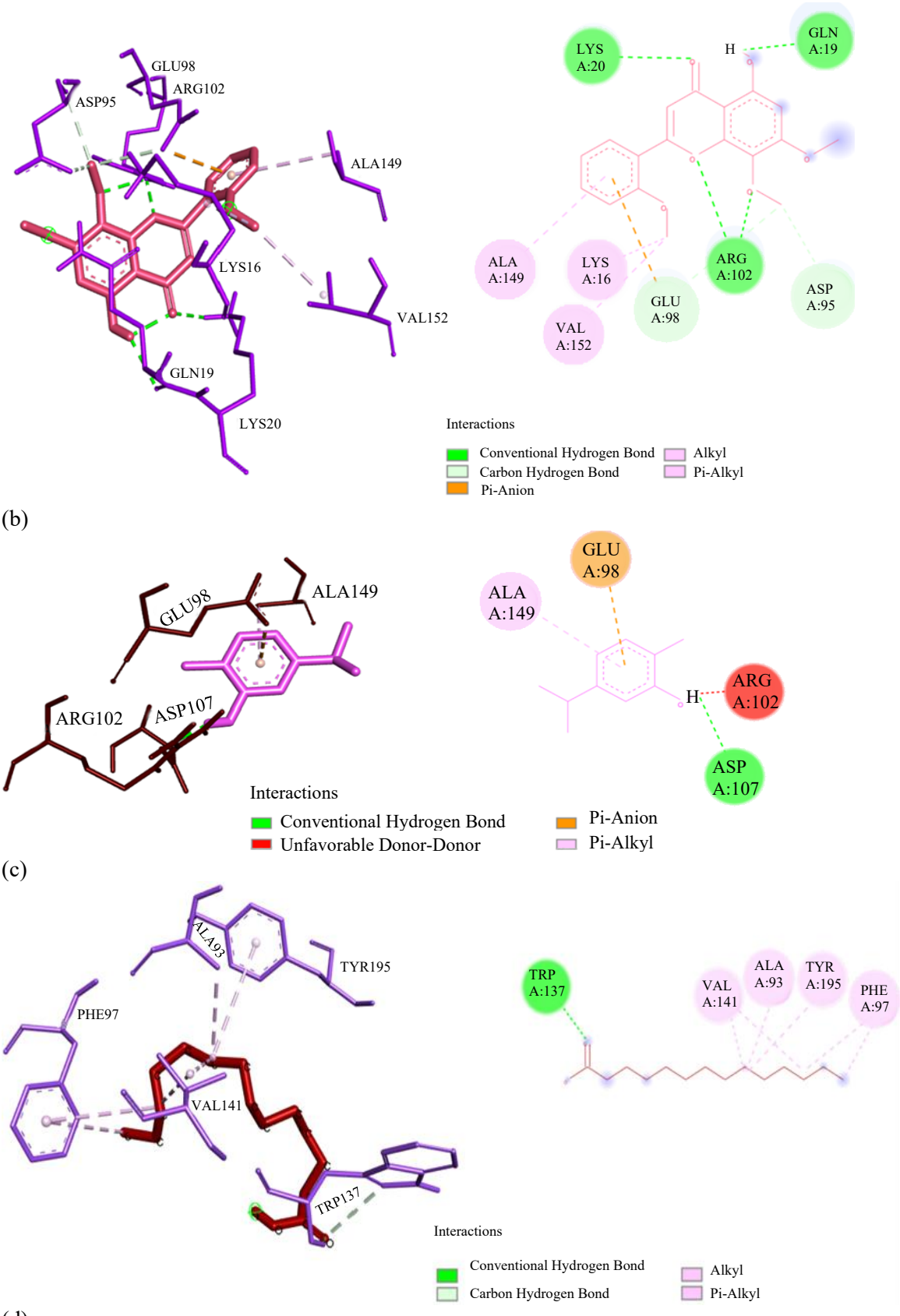
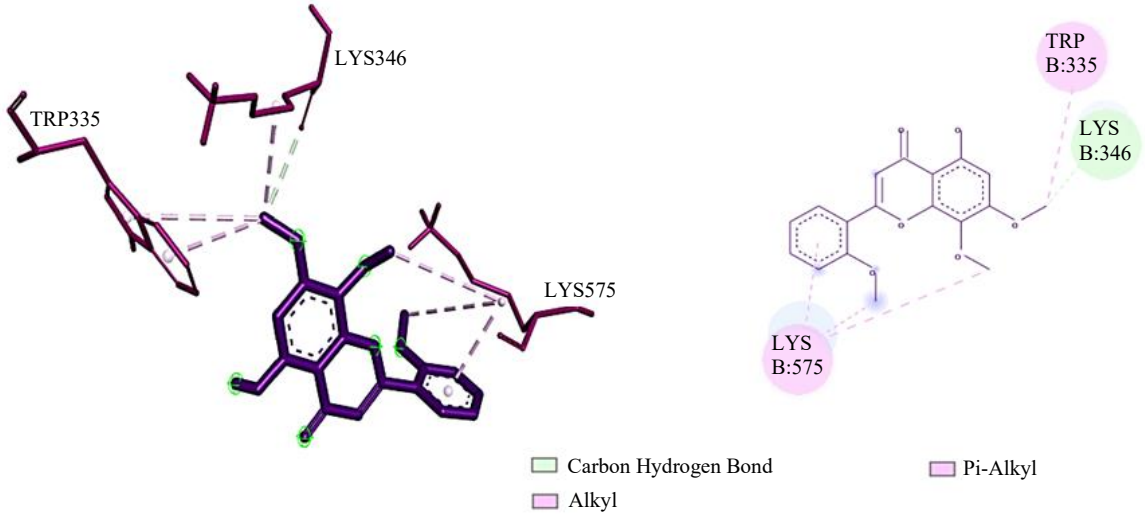


Figure 5. Visualization of 3D and 2D structure molecular interactions of Bcl-xL with ligand, (a.) Andrographin, (b.) 5-Hydroxy-7,8-dimethoxyflavone, (c.) Myristic acid and (d.) Carvacrol.



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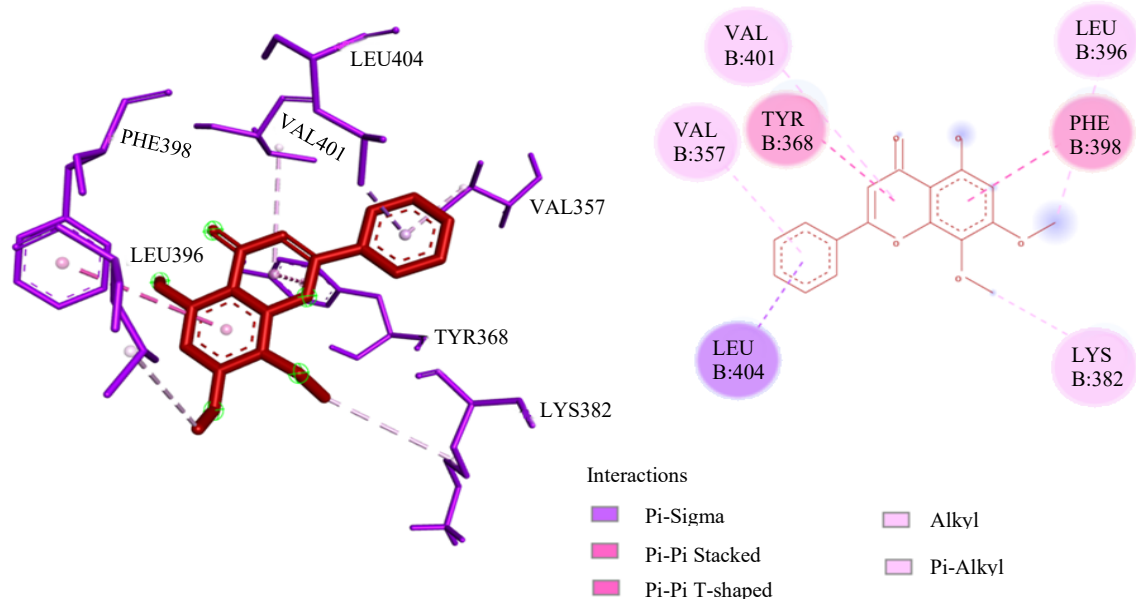

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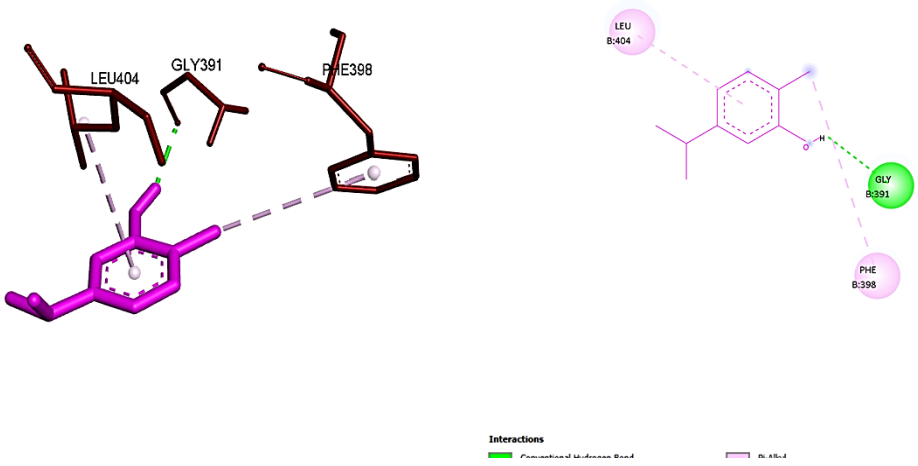

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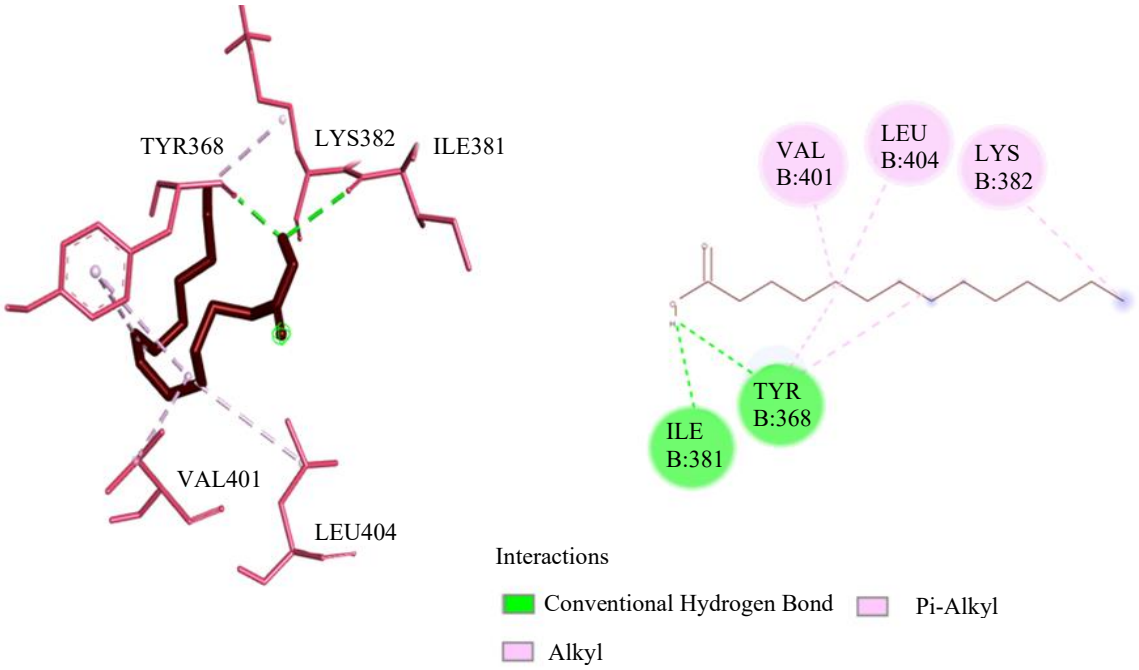

(d)

Figure 6. Visualization of 3D and 2D structure molecular interactions of PI3K with ligands, (a) 5-Hydroxy-7,8-dimethoxyflavone, (b.) Andrographin, (c.) Myristic acid and (d.) carvacrol.

DISCUSSION

Gliomas were traditionally considered to originate from glial cells; recent studies suggest they may arise from immature glial or stem cells. This was further reinforced by the discovery of glioma-initiating cells, which exhibited characteristics of stem cells, including self-renewal and differentiation [22]. Around 80% of malignant brain tumors are of the glioblastoma multiform (GBM) subtype, which is the most common and aggressive. Recent studies have focused on their many biological origins, including stem-like cells, oligodendrocytes, and astrocytes, as well as complex genetic disorders, which together explain their variety and poor prognosis [23].

The Lipinski Rule of 5 is a fundamental guideline for assessing the potential of drug compounds. According to this rule, a drug should have a molecular weight from 150 to 500 Daltons. Its lipophilicity should be less than 4.15. It should have fewer than 5 hydrogen bond donors and fewer than 10 hydrogen bond acceptors. The molar refractivity should be between 40 and 130 $Å^2$. The top four ligands were evaluated based on Lipinski's criteria, and all met the parameters without any breaches [24].

Drug-likeness is influenced by gastrointestinal (GI) absorption, bioavailability, and toxicity, and in this context, blood-brain barrier permeability must also be considered. GI absorption is critical, as the therapeutic effect depends on the drug candidate's ability to dissolve, permeate the intestinal membrane, and reach systemic circulation [25]. Bioavailability refers to the proportion of an administered compound that enters systemic circulation and ideally should exceed 85% to ensure an effective therapeutic response [26]. In addition, the selected phytocompounds must be able to cross the blood–brain barrier, since the present work addresses a neural disorder and effective treatment depends on their ability to reach the central nervous system [27]. the phytocompounds Molecular docking results play a key role by simulating and predicting how ligands interact with target proteins. Docking provides information about binding orientation, affinity, and the stability of complexes. These insights clarify the molecular basis of biological activity and drug–target recognition. In situ, such analysis shows how small molecules occupy binding pockets under near-physiological conditions. This supports rational drug design and validates potential leads before expensive assays. Docking thus helps bridge computational predictions with experimental validation [28, 29].

CONCLUSION

In this study, in silico molecular docking was used to investigate the possible therapeutic benefits of *Andrographis paniculata* in the treatment of gliomas and glioneuronal malignancies. The results offered promising proof that particular phytochemicals from *Andrographis paniculata* might bind to important proteins like PI3K and Bcl-xL, which are both closely linked to the growth and survival of tumors. Although the findings provide a helpful starting point, they are merely the first stage of a much longer process to turn plant-derived chemicals into therapeutically effective treatments.

Molecular dynamics simulations, which can offer a greater understanding of the stability, conformational changes, and long-term interactions of the protein–ligand complexes under physiological settings, should be used in future studies to expand on this work. These simulations would be useful in verifying if the binding seen in docking tests holds up over time and in various environmental conditions. In addition to computer studies, laboratory experiments are crucial. The anticipated inhibitory effects of *Andrographis paniculata* phytochemicals might be confirmed by in vitro tests employing glioma or glioneuronal tumor cell lines, which would also examine the effects of these phytochemicals on cell migration, apoptosis, and proliferation. Additionally, these tests would assist in identifying safe and efficient concentrations.

In the end, pharmacokinetics, bioavailability, and toxicity profiles would need to be evaluated through in vivo research in appropriate animal models. The drugs may advance to preclinical and clinical studies if these phases yield positive results. Therefore, more research combining computational, laboratory, and translational approaches is essential to establish *Andrographis paniculata* as a potential therapeutic option for gliomas and glioneuronal malignancies, even though this study offers encouraging preliminary findings.

Abbreviation

Abbreviation	Full Form
1. ACS	American Chemical Society
2. ADME	Absorption, Distribution, Metabolism, Excretion
3. ALA	Alanine
4. APJCP	Asian Pacific Journal of Cancer Prevention
5. ARG	Arginine
6. ASP	Aspartic acid
7. BIOVIA	Dassault Systèmes BIOVIA Discovery Studio
8. BRAF	v-Raf murine sarcoma viral oncogene homolog B
9. CDK4	Cyclin-Dependent Kinase 4
10. DGONC	Diffuse Glioneuronal Tumor with Oligodendroglioma-like Features and Nuclear Clusters
11. DS	Discovery Studio
12. FGFR2	Fibroblast Growth Factor Receptor 2
13. GBM	Glioblastoma Multiforme
14. GI	Gastrointestinal
15. GLN	Glutamine
16. GLU	Glutamic acid
17. ID	Identification (used in PDB ID)
18. IL	Interleukin
19. IMPPAT	Indian Medicinal Plants, Phytochemistry and Therapeutics database
20. LEU	Leucine
21. LIPINSKI	Lipinski's Rule of Five
22. LYS	Lysine
23. MGT	Myxoid Glioneuronal Tumor

24. MS	Mass Spectrometry
25. MVNT	Multinodular and Vacuolating Neuronal Tumor
26. OPENBABEL	Open Babel chemical toolbox
27. PAINS	Pan-Assay INterference Structure
28. PDB	Protein Data Bank
29. PDBSUM	Protein Data Bank Summary Tool
30. PDGFRA	Platelet-Derived Growth Factor Receptor Alpha
31. PHE	Phenylalanine
32. PLNTY	Polymorphous Low-Grade Neuroepithelial Tumor of the Young
33. PTEN	Phosphatase and Tensin Homolog
34. RCSB	Research Collaboratory for Structural Bioinformatics
35. SDF	Structure Data File (chemical file format)
36. SMILES	Simplified Molecular Input Line Entry System
37. TNF	Tumor Necrosis Factor
38. TRY	Tyrosine
39. VAL	Valine
40. VEGF	Vascular Endothelial Growth Factor
41. WHO	World Health Organization

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