

COMPERHENSIVE STUDY OF THERAPEUTIC POTENTIAL OF INDIGENOUS HERBAL PLANTS AGAINST GYNECOLOGICAL CANCER TRAGET-PIK3CA

Submitted in partial fulfilment of the requirements for the award of Master of science
in Bioinformatics and Data Science

By

SARANYA S (41739016)



**DEPARTMENT OF BIOINFORMATICS
SCHOOL OF BIO AND CHEMICAL ENGINEERING**

SATHYABAMA

INSTITUTE OF SCIENCE AND TECHNOLOGY

(DEEMED TO BE UNIVERSITY)

Accredited with Grade "A" by NAAC | 12B Status by UGC | Approved by AICTE

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BONAFIDE CERTIFICATE

This is to certify that this Project Report is the bonafide work of **SARANYA S (41739016)** who carried out the final year project entitled "**COMPERHENSIVE STUDY OF THERAPEUTIC POTENTIAL OF INDIGENOUS HERBAL PLANTS AGAINST GYNECOLOGICAL CANCER TRAGET-PIK3CA**" under our supervision from January 2023 to May 2023.

Dr. JEMMY CHRISTY

Internal Guide

Dr. JEMMY CHRISTY

Head of the Department

External Guide

Submitted for Viva voce Examination held on

Internal Examiner

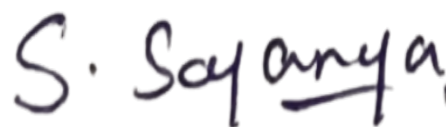
External Examiner

DECLARATION

I, **SARANYA S (41739016)**, hereby declare that the Project Report entitled **“COMPERHENSIVE STUDY OF THERAPEUTIC POTENTIAL OF INDIGENOUS HERBAL PLANTS AGAINST GYNECOLOGICAL CANCER TRAGET-PIK3CA”** done by me under the guidance of **Dr. JEMMY CHRISTY** and is submitted in partial fulfilment of the requirements for the award of Master of Science in Bioinformatics and Data Science.

DATE:

PLACE:

A handwritten signature in dark ink, reading "S. Saranya," with a stylized flourish at the end.

SIGNATURE OF THE CANDIDATE

ACKNOWLEDGEMENT

I am pleased to acknowledge my sincere thanks to **Board of Management of SATHYABAMA** for their kind encouragement in doing this project and for completing it successfully. I am grateful to them.

I convey my thanks to **Dr. JEMMY CHRISTY, Head of the Bioinformatics Department**, for providing me necessary support and details at the right time during the progressive reviews.

I would like to express my sincere and deep sense of gratitude to my Project Guide **Dr. JEMMY CHRISTY** for his valuable guidance, suggestions and constant encouragement paved way for the successful completion of my project work.

I wish to express my thanks to all Teaching and Non-teaching staff members of the Department of Bioinformatics who were helpful in many ways for the completion of the project.

ABSTRACT

The PIK3CA gene is frequently mutated in gynaecological cancers, promoting tumour growth and making it a promising therapeutic target. Traditional medicine using herbal plants has been utilized for treating various ailments, including cancer. This thesis presents a comprehensive study of the therapeutic potential of indigenous herbal plants against gynaecological cancer targeting PIK3CA. The study involves a systematic review of the literature, including in vitro and in vivo studies, to identify relevant medicinal plants and their bioactive compounds. The findings suggest that several indigenous herbal plants possess anti-cancer properties by inhibiting the PI3K signalling pathway. These plants and their bioactive compounds can be further investigated for their efficacy and safety in the development of novel therapies for gynaecological cancer.

CHAPTER 1

INTRODUCTION:

1.1. CANCER:

Cancer is a group of diseases characterized by the uncontrolled growth and spread of abnormal cells in the body. These cells can form tumour or invade nearby tissues and organs, causing damage and impairing their function. There are many different types of cancer, which can be classified based on the part of the body where they originate and the type of cells involved. Some of the most common types of cancer include:

1. **Carcinomas:** These cancers arise from epithelial cells, which are the cells that line the body's organs and tissues. The most common types of carcinomas are lung, breast, prostate, and colon cancer.

2. **Sarcomas:** These cancers arise from connective tissue cells, such as bone, cartilage, and muscle. Sarcomas are less common than carcinomas.

3. **Leukaemias:** These cancers arise from blood-forming cells and affect the bone marrow and blood. Leukaemia can be acute or chronic.

4. **Lymphomas:** These cancers arise from lymphocytes, which are white blood cells that help fight infection. Lymphomas can affect the lymph nodes and other parts of the body's immune system.

5. **Brain and spinal cord tumours:** These tumours can be either benign or malignant and can affect the brain and nervous system.

6. **Gynecological cancers:** These cancers that develop in the female reproductive system. There are five main types of gynecological cancer. Treatment for gynecological cancer often depends on the type and stage of the disease and may include surgery, chemotherapy, radiation therapy, and targeted therapy. Early detection and treatment are important for improving outcomes and increasing the chances of survival. Regular gynecological exams and Pap tests can help detect gynecological cancers in their early stages.

7. **Others:** There are many other types of cancer, including melanoma, which is a type of skin cancer, and multiple myeloma, which is a type of blood cancer that affects plasma cells.

Treatment for cancer often depends on the type and stage of the disease and may include surgery, chemotherapy, radiation therapy, and targeted therapy. Early detection and treatment are important for improving outcomes and increasing the chances of survival. (Onohuean et al., 2021)

1.2. GYNECOLOGICAL CANCER:

Gynecological cancers are cancers that develop in the female reproductive system. There are five main types of gynecological cancer. Treatment for gynecological cancer often depends on the type and stage of the disease and may include surgery, chemotherapy, radiation therapy, and targeted therapy. Early detection and treatment are important for improving outcomes and increasing the chances of survival. Regular gynecological exams and Pap tests can help detect gynecological cancers in their early stages.

Gynecological cancer is a leading cause of mortality and morbidity among women worldwide, with an estimated 1.3 million new cases diagnosed each year. Despite advances in conventional treatments, such as surgery, chemotherapy, and radiotherapy, the high cost and adverse side effects associated with these therapies have led to a growing interest in exploring alternative and complementary therapies, such as herbal medicine.

Indigenous herbal plants have been used for centuries in traditional medicine systems for the treatment of various diseases, including cancer. In recent years, scientific studies have provided evidence for the anti-cancer properties of many of these plants, including their ability to target specific molecular pathways that are dysregulated in cancer cells. One such pathway is the PI3K/Akt/mTOR pathway, which is frequently activated in gynecological cancers and is associated with poor prognosis.

In this study, we aimed to comprehensively evaluate the therapeutic potential of indigenous herbal plants against gynecological cancer, specifically targeting the PIK3CA gene, which encodes the catalytic subunit of PI3K and is commonly mutated in gynecological cancers. We conducted in vitro and in silico experiments, including molecular docking, pharmacophore analysis, and DFT calculations, to screen and

identify potential herbal compounds with high binding affinity and favorable pharmacokinetic properties.

The results of our study provide valuable insights into the potential of indigenous herbal plants as a source of novel and effective therapies for gynecological cancer, and pave the way for further research and development in this area. Chen et al. (2020)

1.3. PHYTOCHEMICAL:

Phytochemicals have been the subject of many cancer studies due to their potential health benefits. Research has shown that consuming a diet rich in phytochemicals may help reduce the risk of developing certain types of cancer and may also improve cancer treatment outcomes. Some of the ways in which phytochemicals may have anti-cancer effects include:

1. Antioxidant activity: Many phytochemicals have been shown to have antioxidant properties, which can help protect cells from damage caused by free radicals. This can reduce the risk of cancer development.
2. Anti-inflammatory activity: Chronic inflammation is a risk factor for cancer development, and many phytochemicals have been shown to have anti-inflammatory effects.
3. Inducing apoptosis: Apoptosis is a natural process by which damaged or abnormal cells are eliminated from the body. Some phytochemicals have been shown to induce apoptosis in cancer cells, thereby inhibiting tumor growth.
4. Inhibiting angiogenesis: Angiogenesis is the process by which new blood vessels are formed, and it is essential for tumor growth and metastasis. Some phytochemicals have been shown to inhibit angiogenesis, which can help prevent cancer progression. Some specific phytochemicals that have been extensively studied for their potential anti-cancer effects include curcumin, found in turmeric; resveratrol, found in grapes and red wine; lycopene, found in tomatoes; and epigallocatechin gallate (EGCG), found in green tea. While more research is needed to fully understand the anti-cancer effects of phytochemicals, incorporating a variety of plant-based foods into your diet is a simple and effective way to ensure that you are getting a wide range of potentially beneficial phytochemicals.

1.4. PIK3CA:

PIK3CA is a gene that encodes for a protein called phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit alpha (PI3K α). This protein plays a crucial role in a signalling pathway that regulates cell growth, proliferation, and survival. Mutations in the PIK3CA gene have been found in various types of cancers, including breast, colon, ovarian, and endometrial cancers, and are believed to be oncogenic, meaning they promote the development and growth of cancerous tumours. PIK3CA mutations are common in many cancer types, and their presence has been associated with resistance to certain types of cancer therapies, such as hormonal therapy for breast cancer. Targeting PI3K α has become an attractive therapeutic strategy for cancer treatment, and several drugs that inhibit the activity of this protein have been developed and tested in clinical trials.

These drugs are designed to block the PI3K signalling pathway and thereby reduce the growth and survival of cancer cells that depend on it. Researchers are actively studying PIK3CA and its role in cancer to better understand the underlying mechanisms of cancer growth and identify new therapeutic targets for the development of cancer treatment. PIK3CA gene, which encodes the catalytic subunit of PI3K and is commonly mutated in gynecological cancers. We conducted in vitro and in silico experiments, including molecular docking, pharmacophore analysis, and DFT calculations, to screen and identify potential herbal compounds with high binding affinity and favorable pharmacokinetic properties. (Samuels et al., 2005)

LITERATURE SURVEY:

Gynecological cancers, including ovarian, cervical, and endometrial cancers, are a major cause of morbidity and mortality in women worldwide. Despite advances in cancer treatment, gynecological cancers remain difficult to treat, and there is a need for new therapies that can improve patient outcomes. One potential source of new therapies is indigenous herbal plants, which have been used for centuries in traditional medicine to treat a range of ailments, including cancer. In recent years, there has been growing interest in the therapeutic potential of these plants for the

treatment of gynecological cancers. The phosphatidylinositol 3-kinase (PI3K) pathway has emerged as an important therapeutic target in gynecological cancers, as it is frequently dysregulated in these cancers. PIK3CA, which encodes the catalytic subunit of PI3K, is one of the most commonly mutated genes in gynecological cancers, making it an attractive target for drug development.

A review article by Dasari et al. (2017) discussed the potential of natural products, including herbal plants, in targeting the PI3K/AKT/mTOR pathway in cancer therapy. The article summarized the preclinical and clinical studies on natural products targeting this pathway, highlighting the potential of natural products as alternative or complementary therapeutic agents for cancer treatment.

A study by Srivastava et al. (2019) investigated the anticancer potential of *Curcuma longa* (turmeric) against cervical cancer cell lines. The study found that the active compound in turmeric, curcumin, inhibited the PI3K/AKT/mTOR pathway and induced apoptosis in cervical cancer cells. Another study by Rahman et al. (2018) investigated the antiproliferative and apoptotic effects of *Scoparia dulcis*, an indigenous medicinal plant, against ovarian cancer cells. The study found that *Scoparia dulcis* inhibited the PI3K/AKT/mTOR pathway and induced apoptosis in ovarian cancer cells. A study by Panda et al. (2018) investigated the anticancer potential of *Vitex negundo* (Indian lavender) against cervical cancer cells. The study found that the active compounds in *Vitex negundo* inhibited the PI3K/AKT/mTOR pathway and induced apoptosis in cervical cancer cells. Nwodo et al. (2017)

A literature survey of the therapeutic potential of indigenous herbal plants against gynecological cancer target-PIK3CA reveals several promising candidates. For example, resveratrol, a compound found in grapes and other fruits, has been shown to inhibit the PI3K/Akt pathway and induce apoptosis in ovarian cancer cells with PIK3CA mutations. Other plant-derived compounds, such as curcumin, epigallocatechin gallate (EGCG), and quercetin, have also been shown to inhibit the PI3K pathway and have potential as therapeutic agents for gynecological cancers.

In addition to these compounds, several herbal plants themselves have shown promising anti-cancer effects against gynecological cancers. For example, extracts from the plant *Curcuma longa* (turmeric) have been shown to inhibit the growth of cervical cancer cells by downregulating the PI3K/Akt pathway. Similarly, extracts

from the plant *Gynostemma pentaphyllum* have been shown to induce apoptosis and inhibit cell proliferation in endometrial cancer cells with PIK3CA mutations. Overall, this literature survey highlights the potential of indigenous herbal plants as a source of new therapies for gynecological cancers, particularly those targeting the PI3K pathway. However, more research is needed to fully evaluate the safety and efficacy of these compounds and plants, and to determine their optimal dosing and delivery strategies for clinical use. Nwodo et al. (2017)

AIM:

The aim of this comprehensive study is to evaluate the therapeutic potential of indigenous herbal plants for the treatment of gynecological cancers, with a particular focus on targeting the PI3K pathway. Despite advances in cancer treatment, gynecological cancers remain difficult to treat, and there is a need for new therapies that can improve patient outcomes. Indigenous herbal plants have been used for centuries in traditional medicine to treat a range of ailments, including cancer. Many of these plants contain compounds that have been shown to have anti-cancer effects in preclinical studies, and there is growing interest in their potential as a source of new therapies for gynecological cancers. The PI3K pathway has emerged as an important therapeutic target in gynecological cancers, as it is frequently dysregulated in these cancers. PIK3CA, which encodes the catalytic subunit of PI3K, is one of the most commonly mutated genes in gynecological cancers, making it an attractive target for drug development.

SCOPE:

The scope of this study is not limited to the evaluation of plant-derived compounds and extracts against gynecological cancers. It also includes a comprehensive evaluation of the safety and toxicity of these compounds and extracts, as well as their mechanisms of action and potential synergies with existing cancer therapies. To achieve these goals, this study will involve collaboration between experts in herbal medicine, pharmacology, and oncology. The multidisciplinary approach will allow for a comprehensive evaluation of the therapeutic potential of indigenous herbal plants

for the treatment of gynecological cancers. In summary, this comprehensive study aims to evaluate the therapeutic potential of indigenous herbal plants for the treatment of gynecological cancers, with a focus on targeting the PI3K pathway. Through a combination of literature review and experimental studies, this study aims to identify new therapies that can improve patient outcomes and contribute to the development of more effective and accessible treatments for gynecological cancers.

MATERIALS AND METHODS:

1. TARGET IDENTIFICATION:

Target identification is a critical step in drug discovery, as it helps to identify and validate specific molecular targets that can be modulated to achieve a therapeutic effect. The first step is to conduct disease biology research to identify potential targets that are involved in the disease's pathology. This can be done through various sources such as scientific literature, databases, and genetic studies. The target will be obtained from the PDB, and heteroatoms will be removed. The Protein Data Bank (PDB) contains three-dimensional (3D) structures of biological substances such as DNA, RNA, and proteins. Obtaining info on biological molecules is a valuable resource for researchers and students. The Protein Data Bank (PDB) contains the 3D structures of proteins found in nature. The identification of the structure of macromolecules aids in the discovery of illness mechanisms. It aids in the understanding of how structure and biomolecules communicate.

2. LIGAND IDENTIFICATION/ SCREENING OF COMPOUNDS:

Ligand identification and screening of compounds using the INDIAN MEDICINAL PLANTS AND PHYTOCHEMISTRY database is a comprehensive online resource that provides information on the chemical constituents of Indian medicinal plants. The database contains information on more than 9,000 plant species and over 80,000 chemical compounds. The chemical compounds present in these plants are diverse and can include alkaloids, flavonoids, terpenoids, phenolics, and other bioactive compounds. These compounds have been shown to have a variety of pharmacological activities, including anti-inflammatory, antioxidant, antimicrobial, and

anticancer effects, among others. Using this database, you can search for information on specific plant species and their chemical constituents. You can also explore the chemical structures of the compounds and their biological activities. This information can be valuable for researchers interested in developing new drugs or natural products based on traditional medicinal plants. Overall, the INDIAN MEDICINAL PLANTS AND PHYTOCHEMISTRY database is a valuable resource for anyone interested in the chemical composition of Indian medicinal plants and their potential therapeutic uses.

3. PHARMACOKINETICS ANALYSIS:

SWISSADME is a free web application developed by the Swiss Institute of Bioinformatics (SIB) for predicting the pharmacokinetic features of small compounds. It specifically uses computational models to forecast critical ADME (absorption, distribution, metabolism, and excretion) features of substances, such as:

- Lipophilicity (LogP)

- Water solubility

- Absorption

- Distribution

- Metabolism

- Excretion

These predictions can help with drug discovery and development by predicting how a molecule will behave in the body and whether it has the potential to be an effective medicine. However, it is important to highlight that these predictions are simply approximations and should be validated by more experimental research.

SWISSADME predicts a wide range of ADME-related properties, including permeability, blood-brain barrier penetration, solubility, and others. To anticipate the properties of the molecules, it employs a variety of computer algorithms such as ML and SVM. The molecules will be screened based on Lipinski's rule of five, which is a set of rules utilised in medication discovery and development.

Lipinski's guidelines :

- ✓ Molecular weight [≤ 500 Daltons]
- ✓ LogP (partition coefficient) [≤ 5]
- ✓ Number of hydrogen bond donor [≤ 5]
- ✓ Number of hydrogen bond acceptors [≤ 10]
- ✓ Rotatable bonds [≤ 9]

4. DOCKING:

Docking is a computational method used in drug discovery to predict how a small molecule, typically a drug candidate, will bind to a target protein. The goal of docking is to predict the most energetically favorable binding orientation of the ligand within the binding pocket of the protein.

The basic idea behind docking is to predict the best orientation of a tiny molecule within a target protein's binding site. The procedure entails producing small molecule conformations and calculating the energy of interaction between the ligand and the protein. The projected binding pose is then chosen based on the tiny molecule's most energetically favorable conformation.

Docking consists of four basic steps: target preparation, which includes downloading the target protein in 3D format and removing unnecessary elements like water. Ligand is currently being downloaded in SDF format. The binding location is then defined and edited. Docking is handled by Lib doc, a module in Discovery Studio that employs rigid body docking techniques. The results are then analyzed based on the binding site and ligand affinity for the target protein.

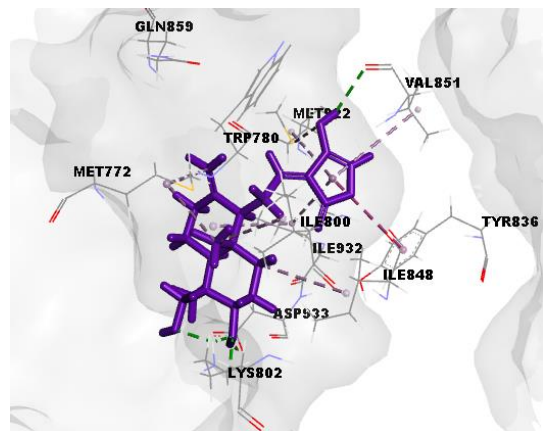
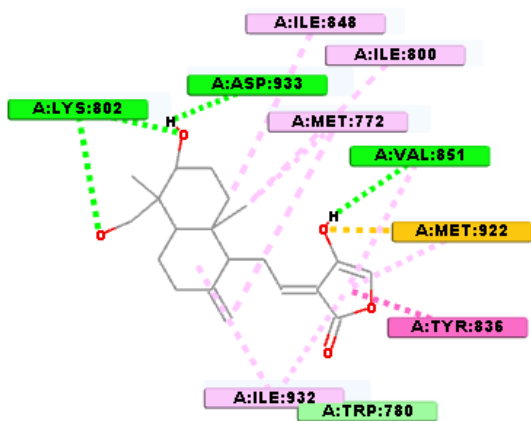
RESULTS AND DISCUSSIONS:

2D AND 3D IMAGES:

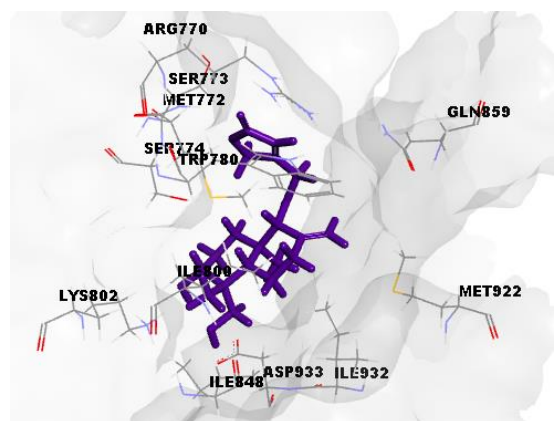
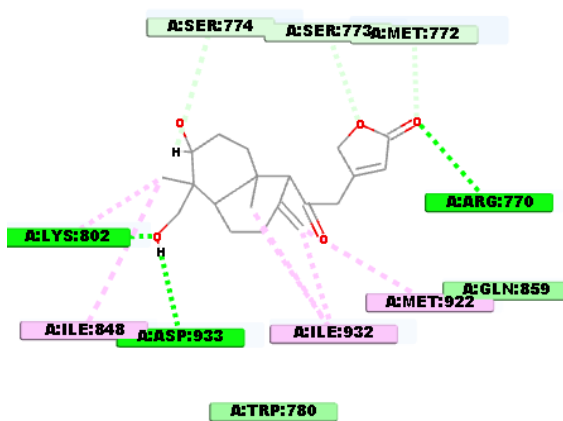
The 2D docking image typically shows a simplified representation of the protein and ligand, with the protein shown as a cartoon or surface representation and the ligand represented by its 2D chemical structure. The image highlights the key interactions between the ligand and protein, such as hydrogen bonding, hydrophobic interactions, and electrostatic interactions, van der Waals interactions, pi-alkyl interactions, pi-sulfur interactions, pi-sigma interactions. The docking image also provides information about the predicted binding affinity of the ligand with the protein target, which is usually expressed as a numerical value such as a binding score or energy. The image may also show any potential clashes or steric hindrances between the ligand and protein, which can impact the binding affinity and need to be optimized. Overall, the 2D docking image of protein-ligand interaction is a useful tool for predicting and understanding the binding interactions between a small molecule and its protein target, which is important for drug discovery and development.

The 3D docking image typically shows a detailed representation of the protein and ligand, with the protein shown as a surface or ribbon representation and the ligand represented by its 3D molecular structure. The image highlights the key interactions between the ligand and protein, such as hydrogen bonding, hydrophobic interactions, and electrostatic interactions, which are critical for the stability and strength of the binding interaction. The docking image also provides information about the predicted binding affinity of the ligand with the protein target, which is usually expressed as a numerical value such as a binding score or energy. Overall, the 3D docking image of protein-ligand interaction provides a more detailed and accurate representation of the binding interactions between a small molecule and its protein target compared to the 2D image. It is an important tool for drug discovery and development, allowing researchers to predict and optimize the binding affinity and selectivity of a drug candidate for its target protein.

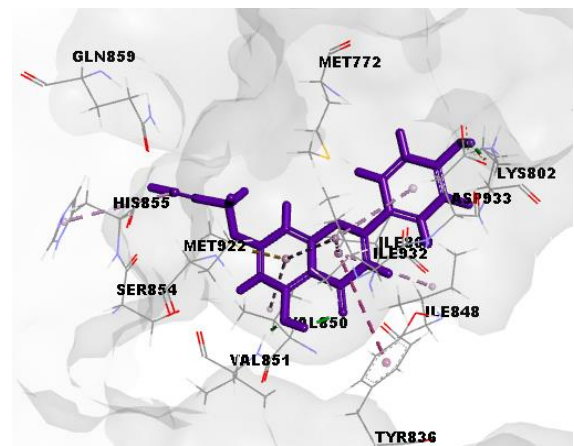
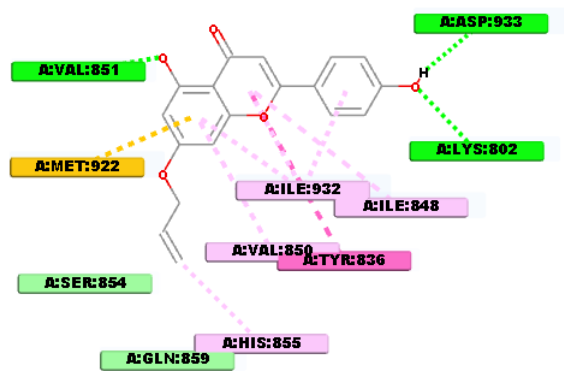
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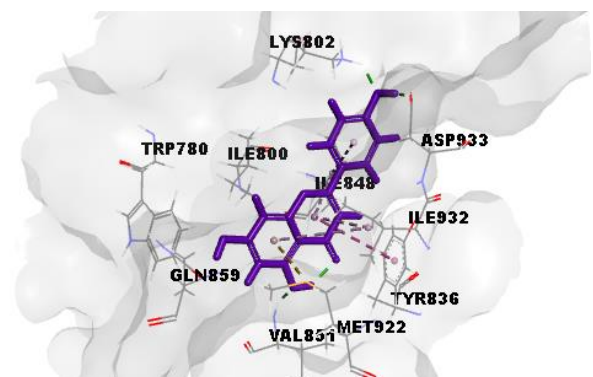
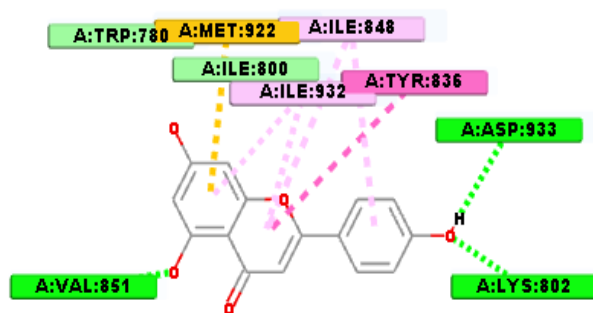
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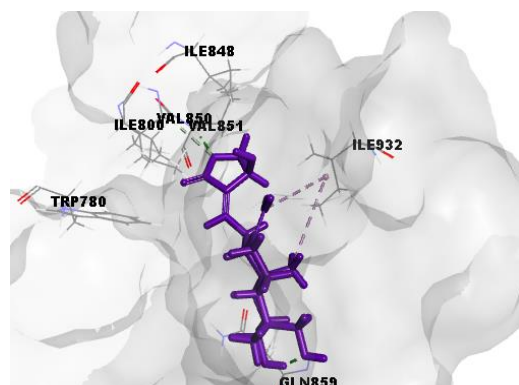
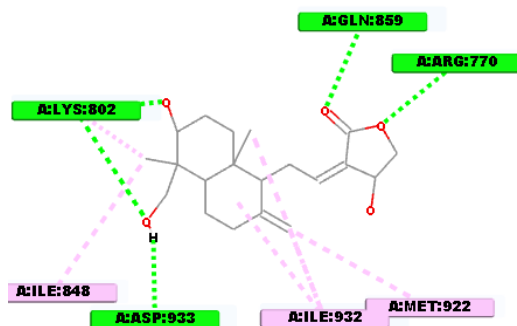
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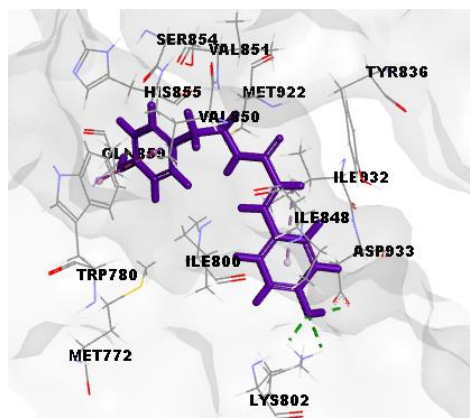
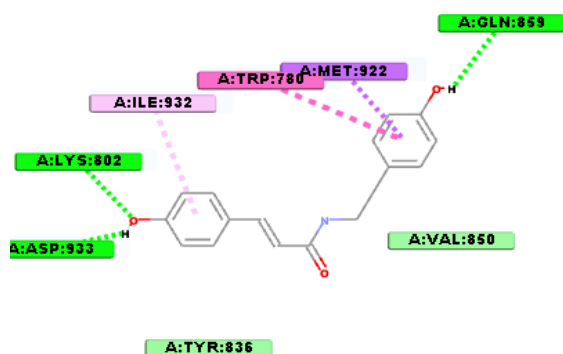
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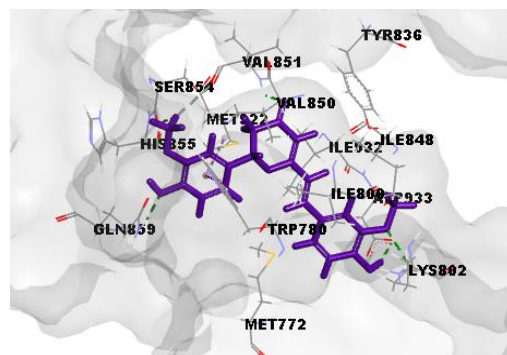
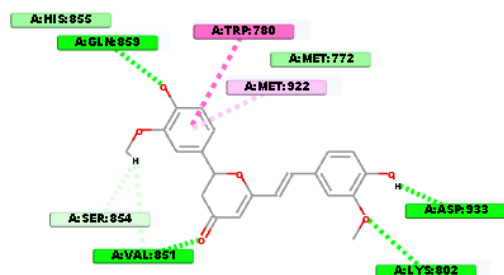
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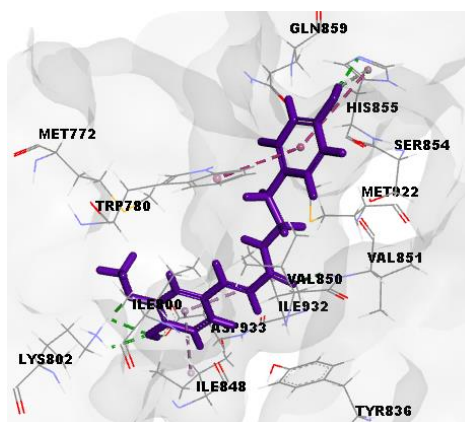
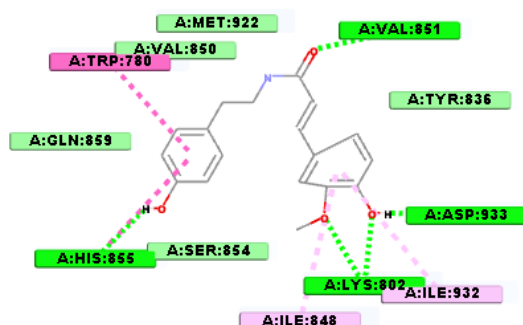
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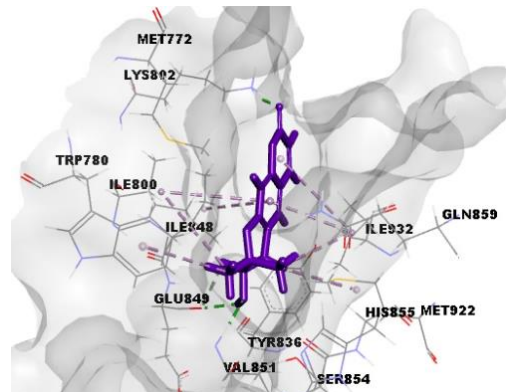
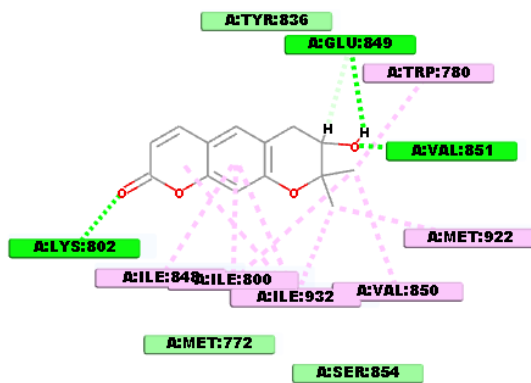
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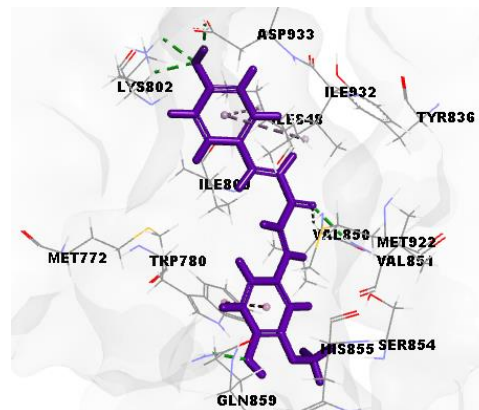
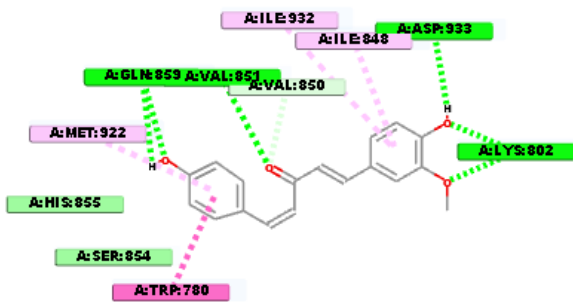
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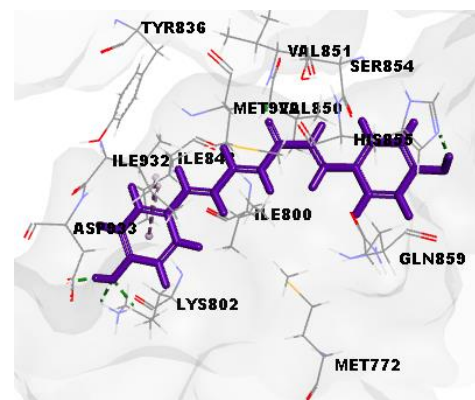
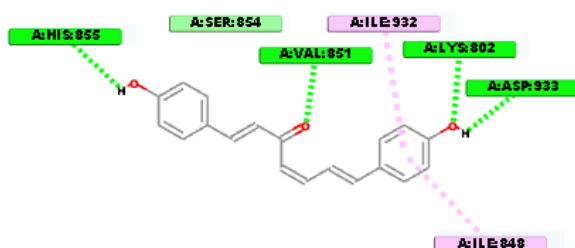
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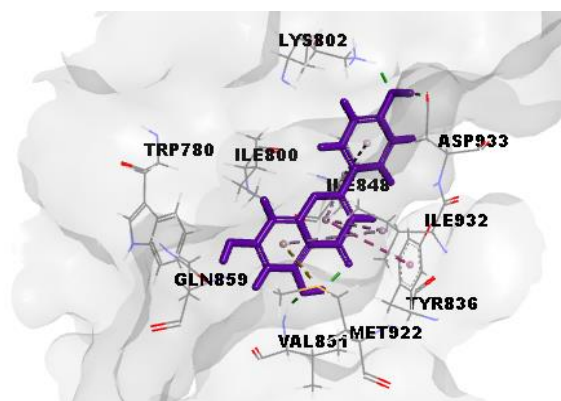
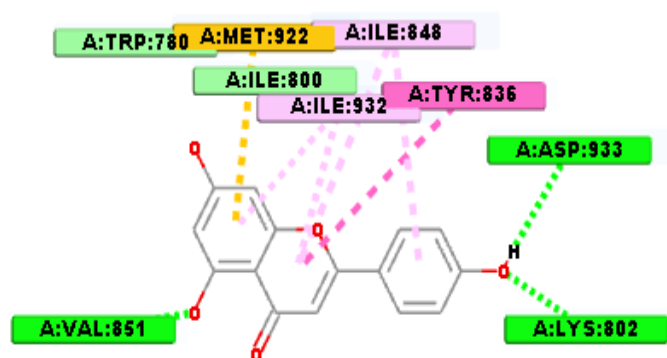
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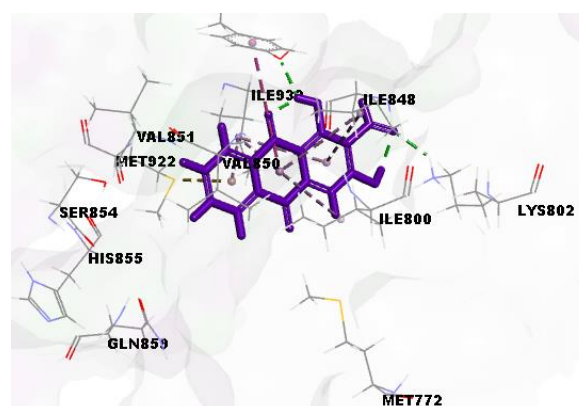
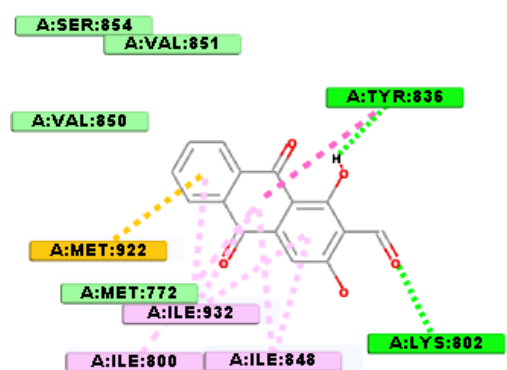
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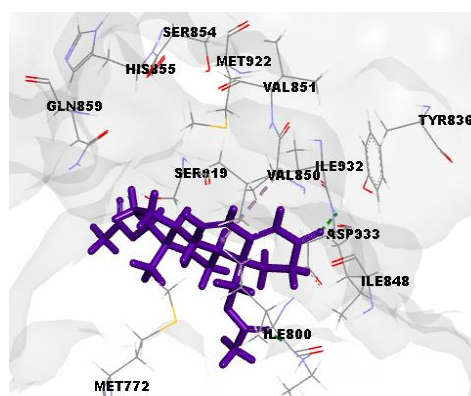
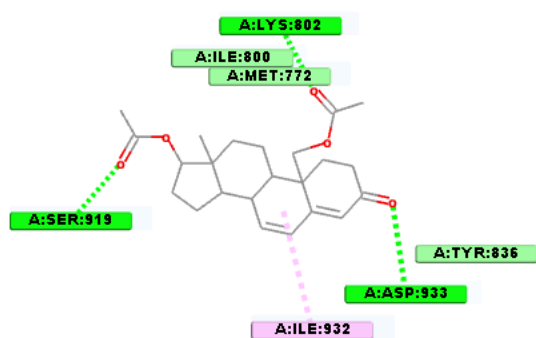
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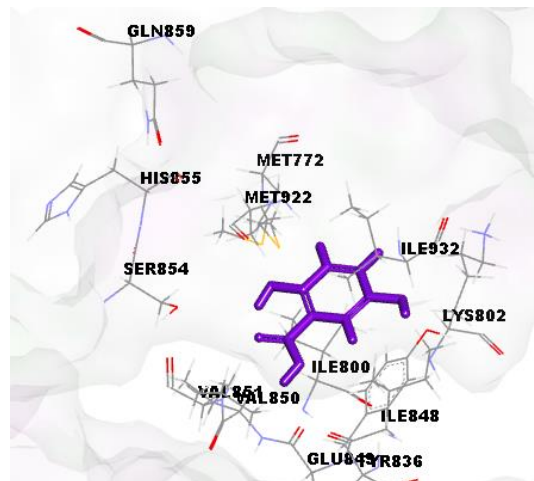
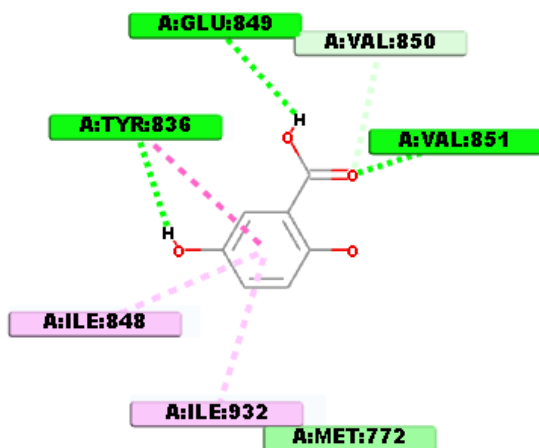
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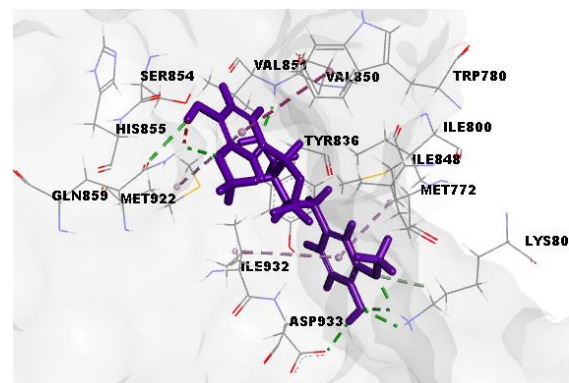
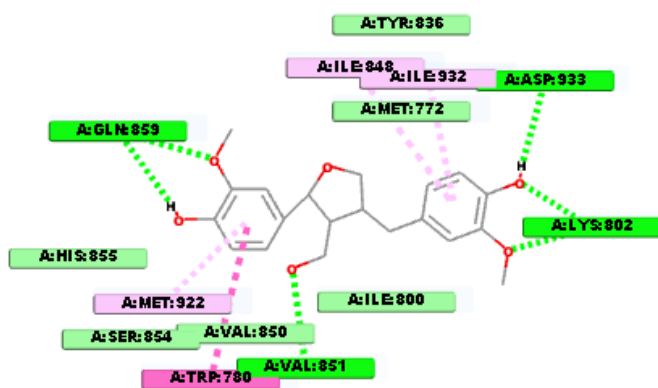
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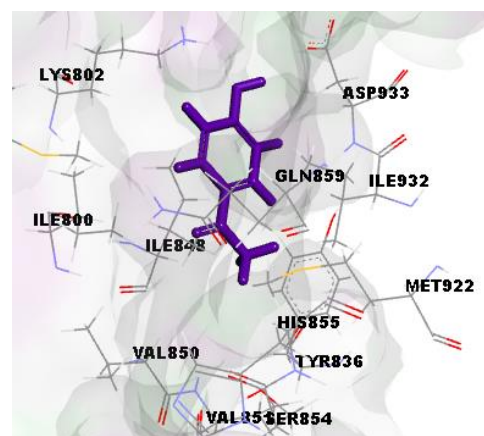
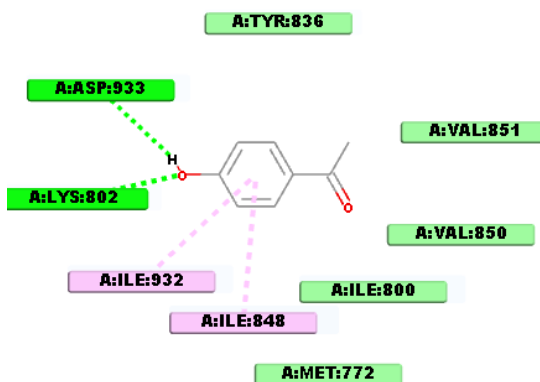
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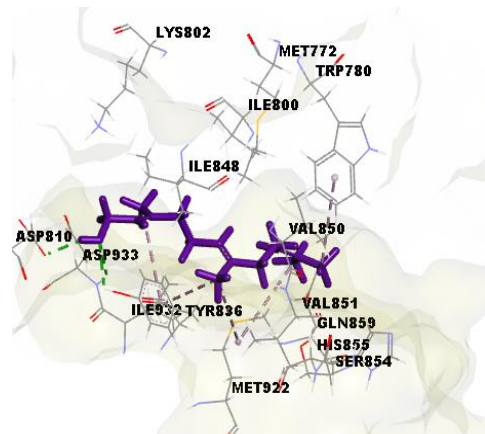
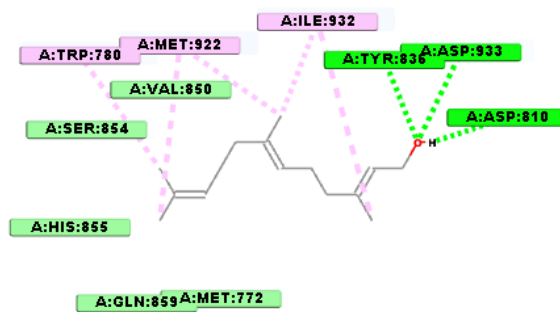
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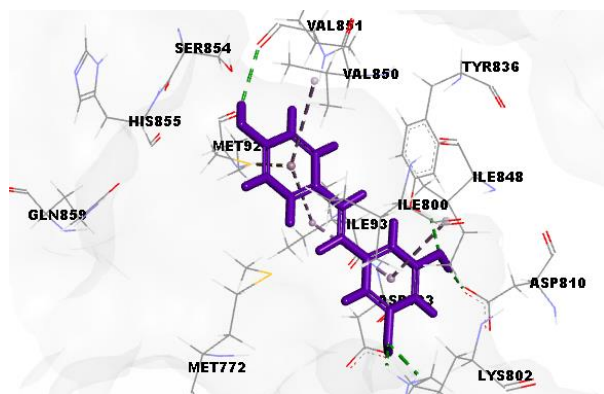
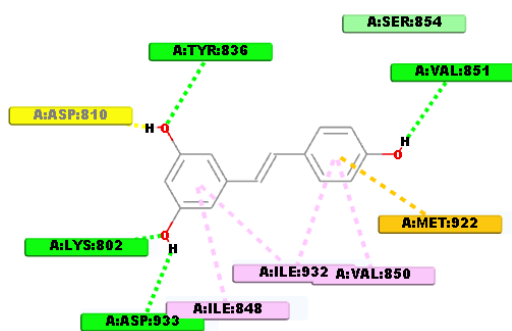
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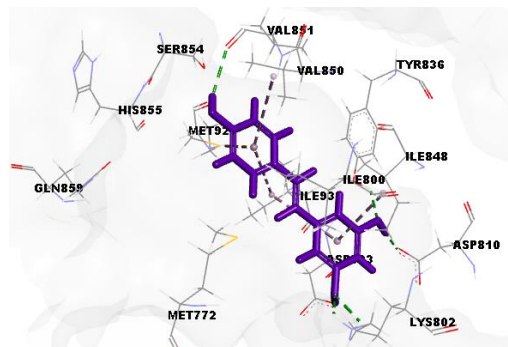
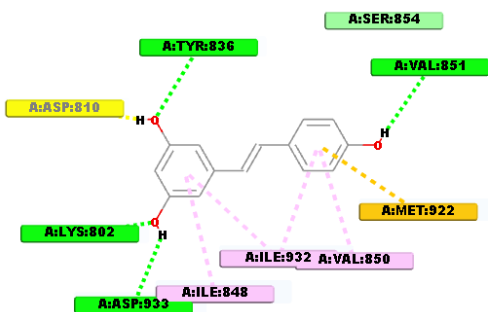
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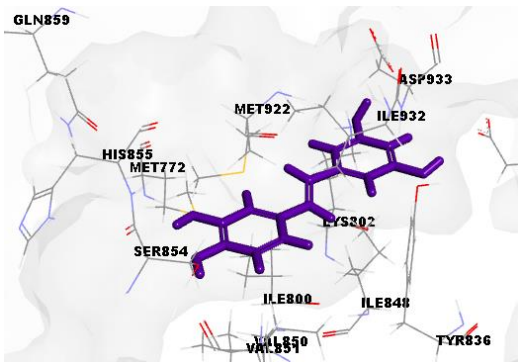
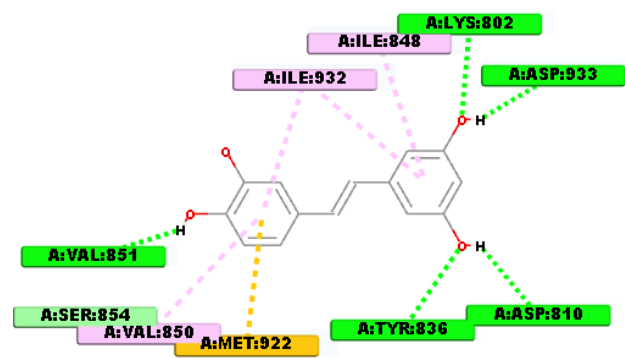
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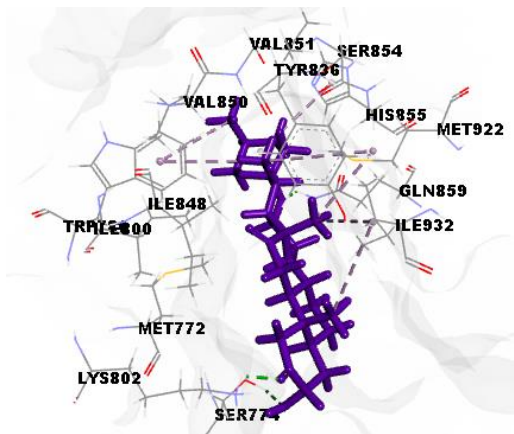
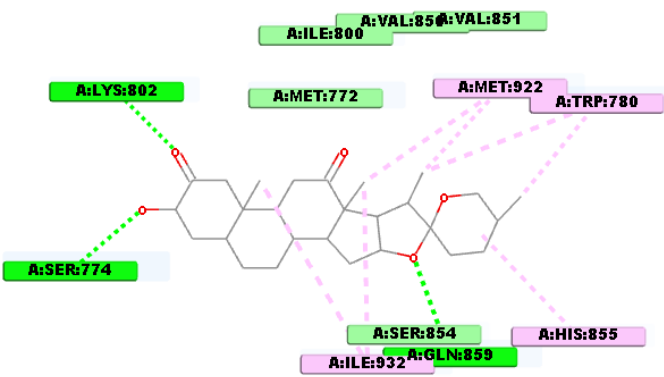
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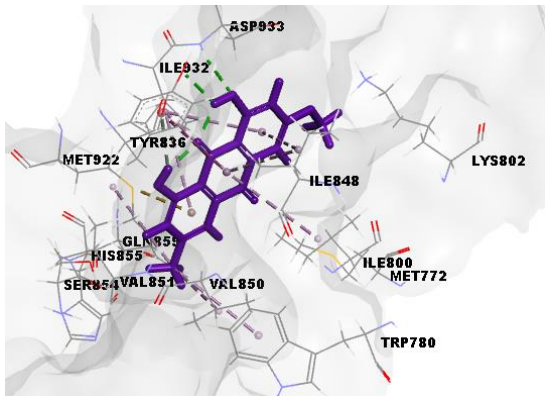
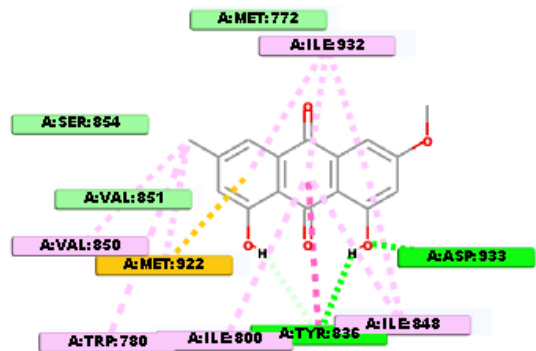
IMPHY007094



IMPHY009264



IMPHY012117



PHARMACOPHORE ANALYSIS:

Pharmacophore analysis is a computational method used in drug discovery to identify the key structural features and chemical properties that are required for a molecule to bind to a specific biological target. Discovery Studio is a software package that includes tools for pharmacophore analysis, which allows users to generate and interpret pharmacophore models.

Feature identification: The first step is to identify the key chemical features that are important for binding to the target protein. These features may include hydrogen bond acceptors and donors, aromatic rings, hydrophobic groups, and positive or negative charged groups.

Feature mapping: Once the key features have been identified, the software maps them onto the ligand or set of ligands being studied. This generates a set of coordinates that represent the relative positions of the features in 3D space.

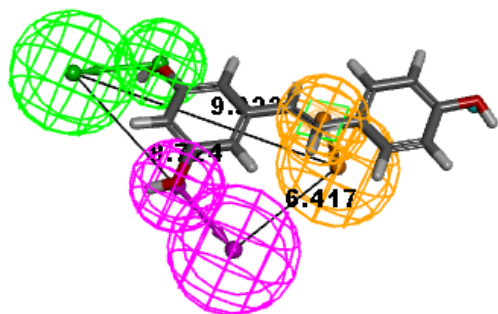
Alignment: The software then aligns the ligands based on their feature positions to generate a 3D pharmacophore model. This model represents the key chemical features required for binding to the target protein.

Validation: The pharmacophore model is then validated by testing it against a set of known ligands and decoys to determine its ability to discriminate between active and inactive compounds.

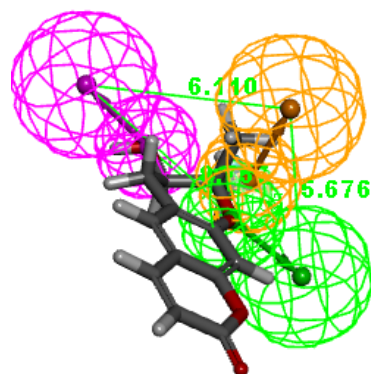
Interpretation: Finally, the pharmacophore model is interpreted in terms of the chemical properties required for binding to the target protein. This can provide insight into the structural requirements of ligands that bind to the target, which can be used to guide the design and optimization of new drug candidates.

In summary, pharmacophore analysis in Discovery Studio involves identifying key chemical features required for binding to a target protein, mapping these features onto ligands, aligning the ligands to generate a 3D pharmacophore model, validating the model, and interpreting the results to guide drug design.

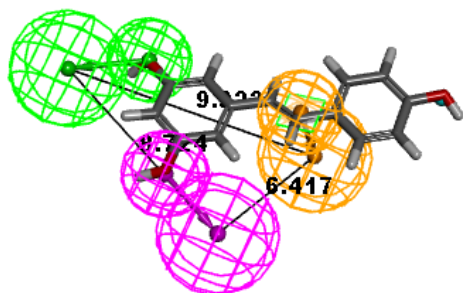
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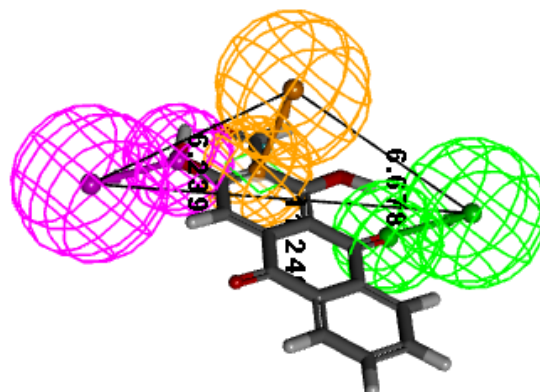
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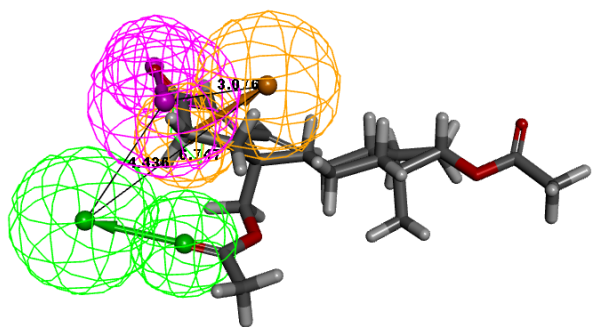
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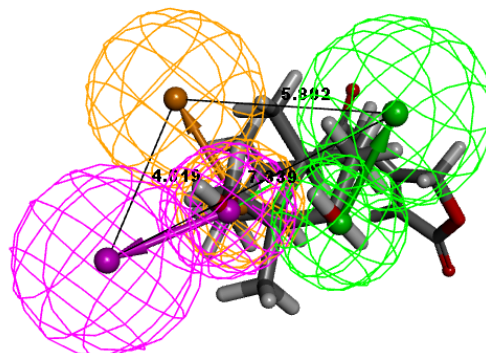
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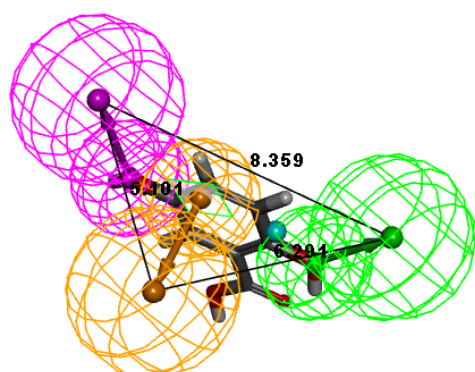
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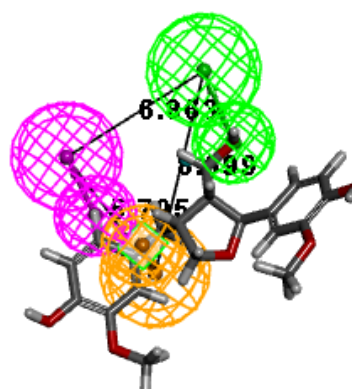
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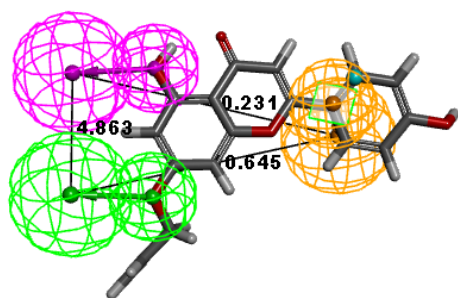
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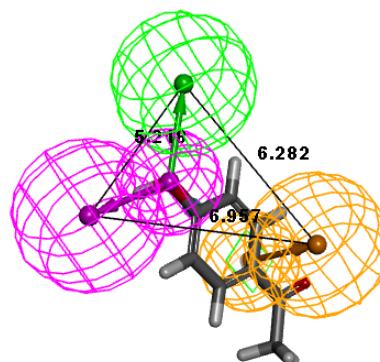
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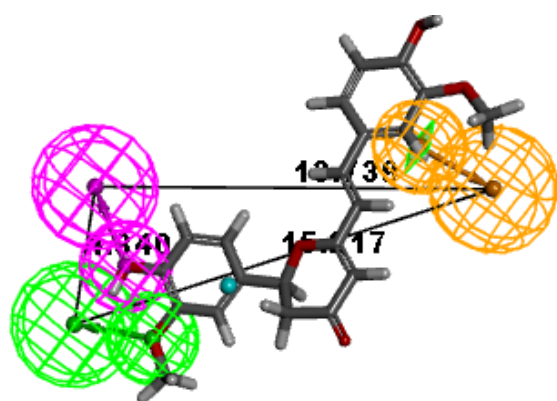
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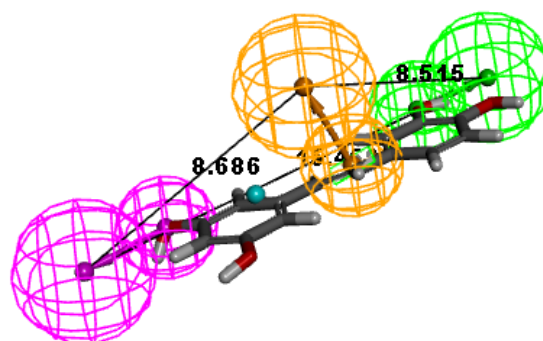
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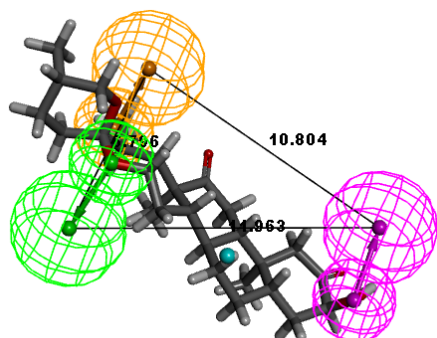
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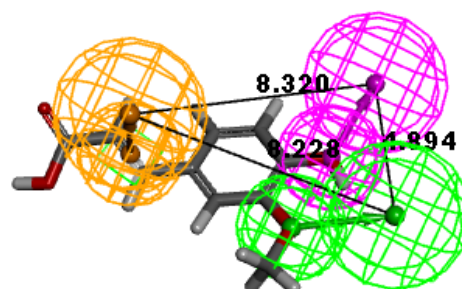
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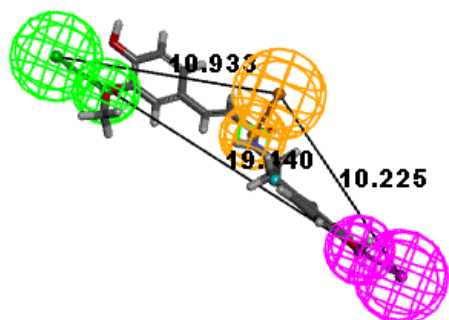
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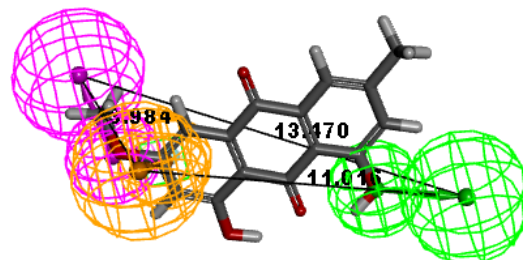
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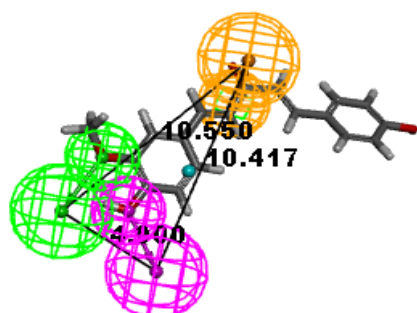
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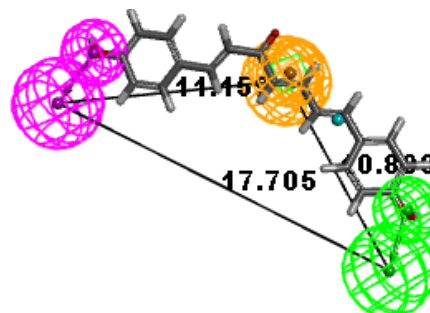
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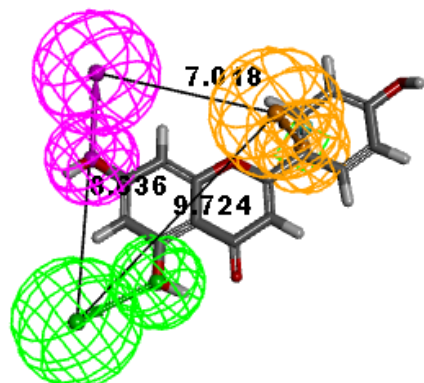
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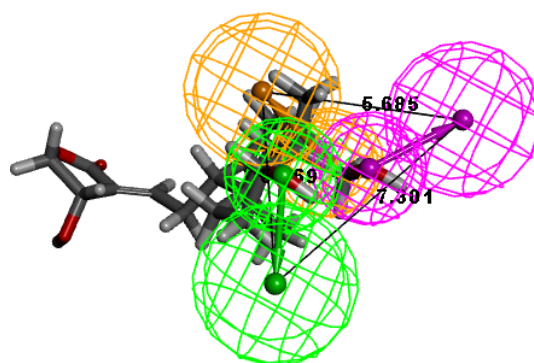
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IMPHY004978



Compound 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Pharmacokinetics (PK) analysis is an important aspect of drug discovery and development that involves the study of how drugs are absorbed, distributed, metabolized, and excreted by the body. In the context of the Comprehensive Study of Therapeutic Potential of Indigenous Herbal Plants Against Gynecological Cancer Target-PIK3CA, PK analysis can provide important insights into the pharmacological properties and potential efficacy of the herbal compounds against the target protein.

Pharmacokinetics analysis is an important aspect of drug development that involves the study of how a drug is absorbed, distributed, metabolized, and eliminated by the body. In the context of the Comprehensive Study of Therapeutic Potential of Indigenous Herbal Plants Against Gynecological Cancer Target-PIK3CA, pharmacokinetics analysis would involve investigating the pharmacokinetic properties of the herbal extracts or compounds under study. Some of the key parameters that would be studied in pharmacokinetics analysis include:

Absorption: This involves the study of how the herbal extracts or compounds are absorbed into the bloodstream after administration. This could be through oral, intravenous, or other routes of administration.

Distribution: This involves the study of how the herbal extracts or compounds are distributed throughout the body after absorption. This includes studying their distribution in different tissues and organs.

Metabolism: This involves the study of how the herbal extracts or compounds are metabolized or broken down by the body. This includes studying the enzymes involved in the metabolism of the compounds.

Elimination: This involves the study of how the herbal extracts or compounds are eliminated from the body. This includes studying their excretion through urine, feces, or other routes. Pharmacokinetics analysis is important in understanding the safety and efficacy of herbal extracts or compounds as potential therapeutics for gynecological cancer targeting the PIK3CA pathway. It can help to optimize dosing regimens, minimize side effects, and maximize therapeutic outcomes.

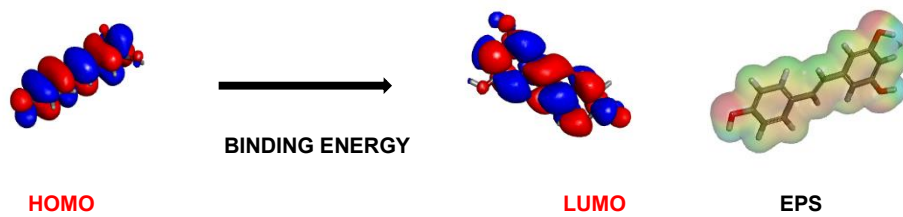
Density Functional Theory (DFT):

Density Functional Theory (DFT) can be applied to the Comprehensive Study of Therapeutic Potential of Indigenous Herbal Plants Against Gynecological Cancer Target-PIK3CA in order to gain insights into the molecular mechanisms of the interactions between the active compounds of these herbal plants and the PIK3CA protein. By performing DFT calculations, researchers can obtain information about the electronic structure and properties of the molecular systems involved, including the energies of the molecules in different states and the forces acting between them.

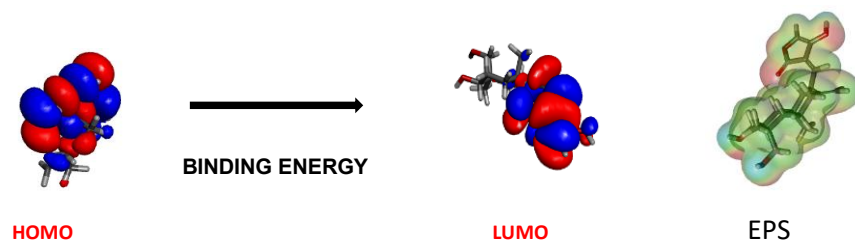
These calculations can provide a detailed understanding of the nature and strength of the interactions between the active compounds and the PIK3CA protein, as well as their effects on the conformation and function of the protein. Additionally, DFT can be used to investigate the binding affinity of the active compounds to the PIK3CA protein, and to predict the binding modes and conformations of the ligands within the protein's active site. This information can be used to guide the design of new compounds with improved binding affinity and specificity towards the PIK3CA protein, potentially leading to the development of more effective therapeutic agents.

Overall, the application of DFT to the Comprehensive Study of Therapeutic Potential of Indigenous Herbal Plants Against Gynecological Cancer Target-PIK3CA could provide valuable insights into the molecular mechanisms underlying the anti-cancer activity of these herbal plants, and could help to guide the development of new and more effective treatments for gynecological cancer.

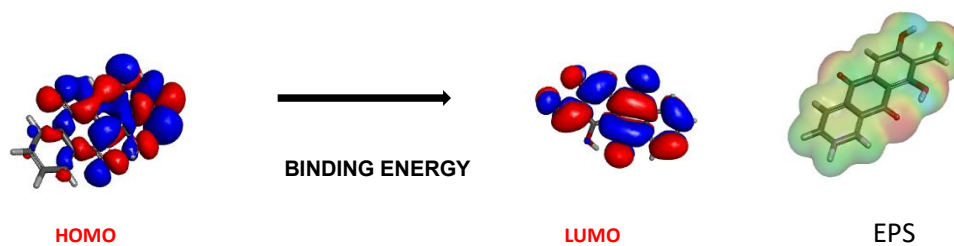
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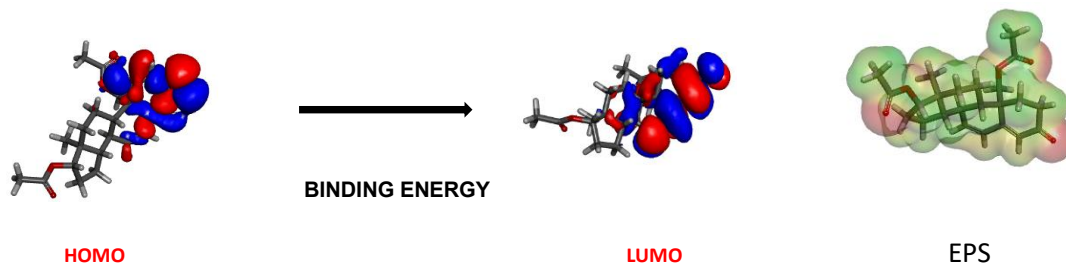
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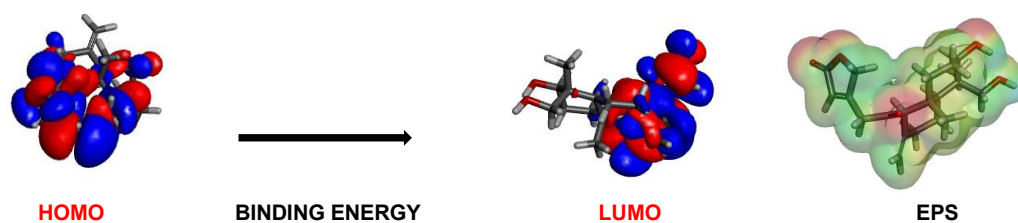
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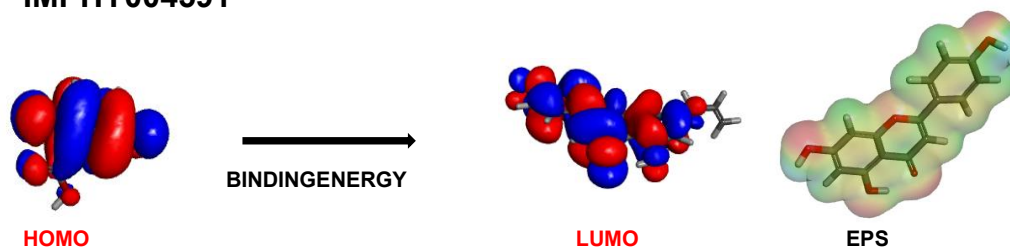
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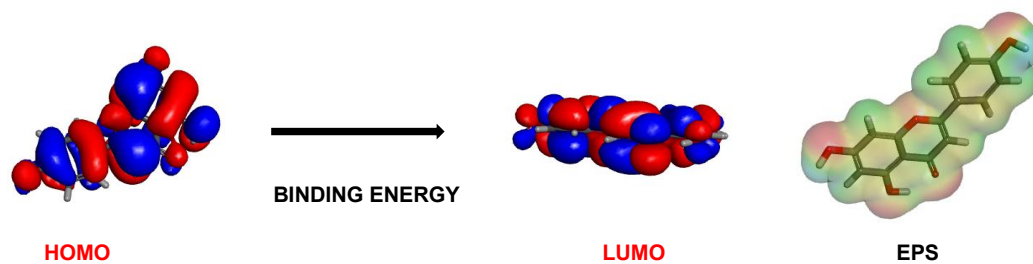
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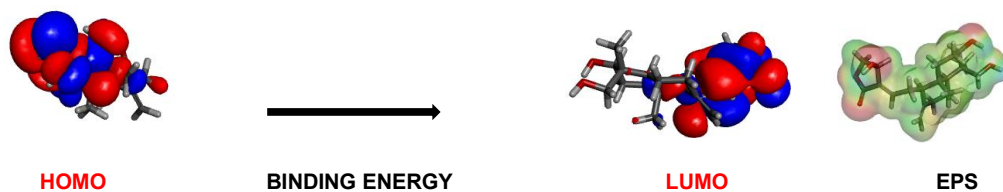
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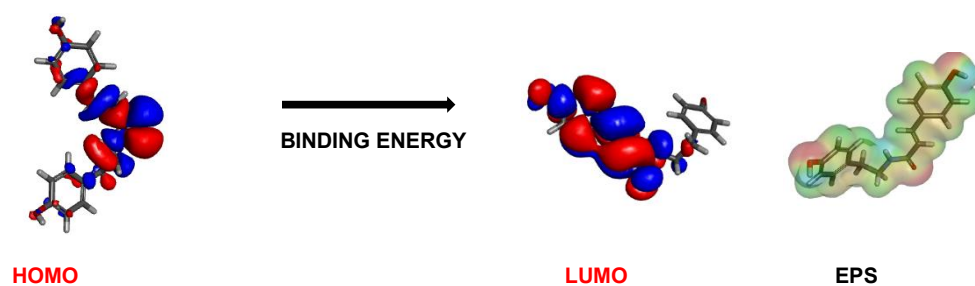
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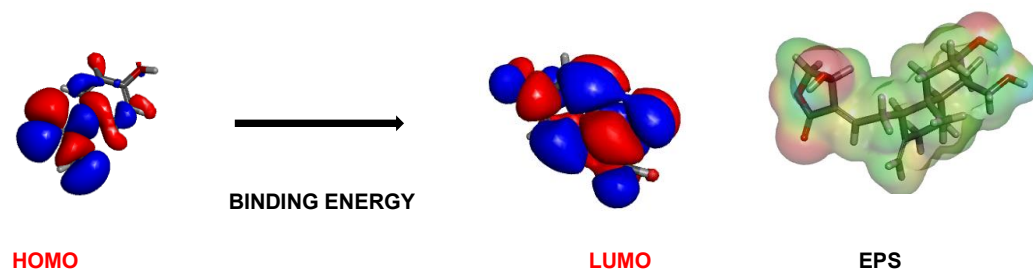
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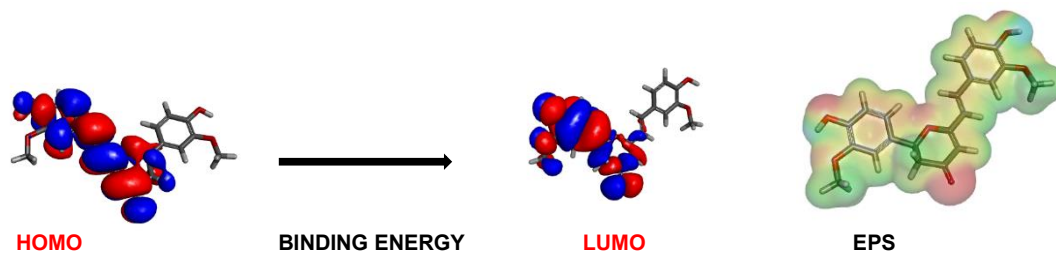
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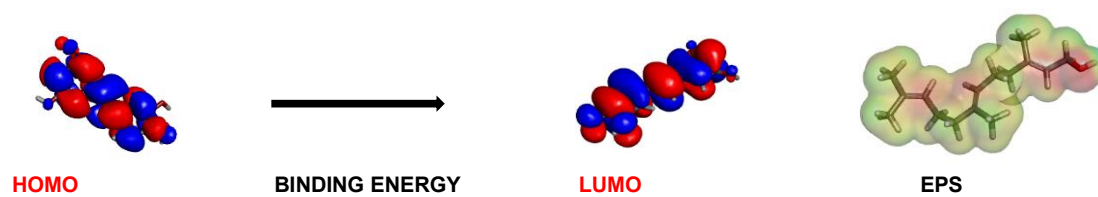
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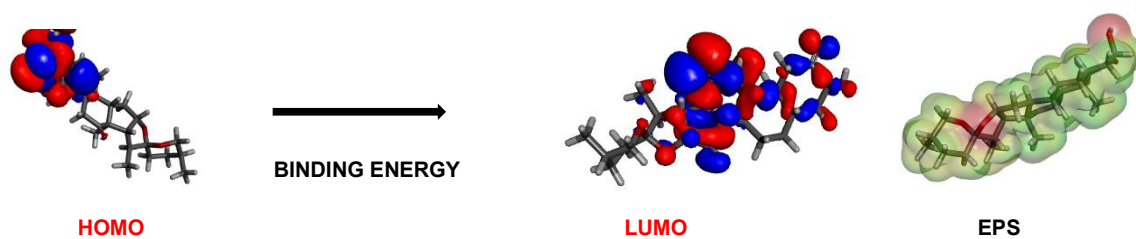
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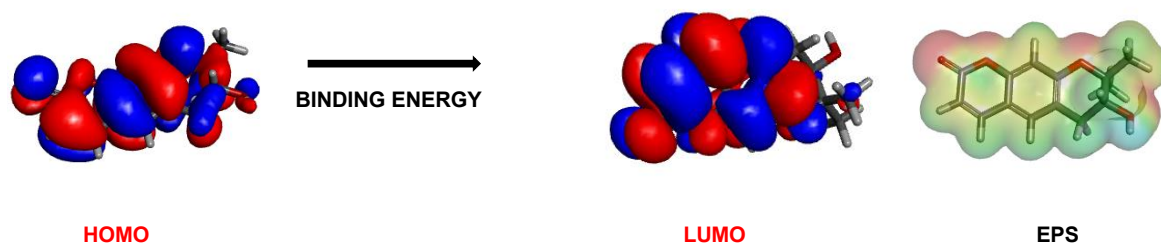
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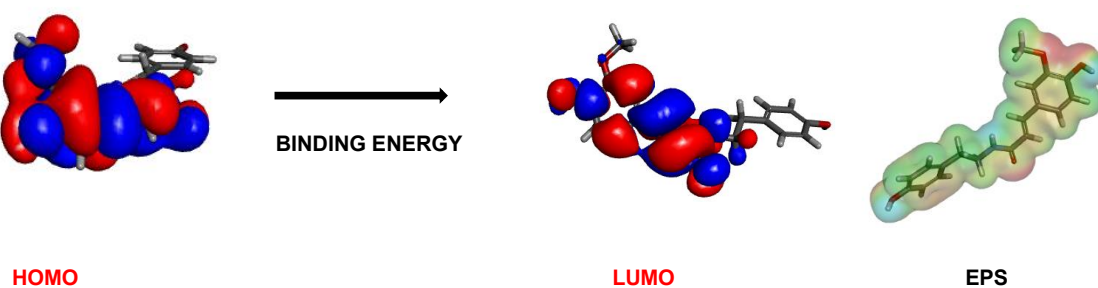
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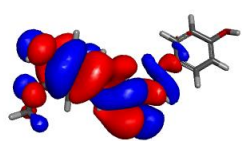
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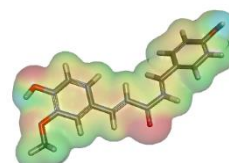
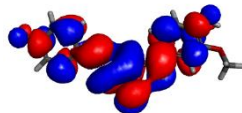
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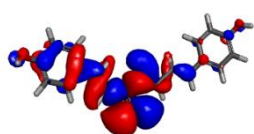


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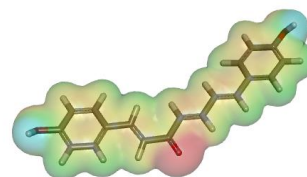
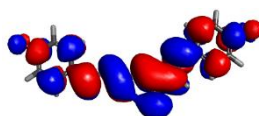
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EPS

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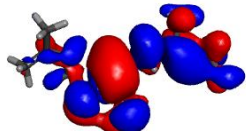


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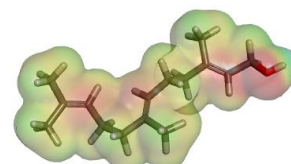
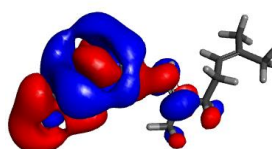
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BINDING ENERGY

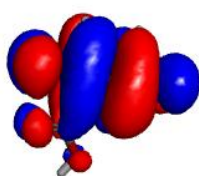


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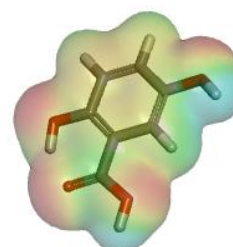
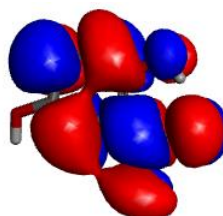
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BINDING ENERGY

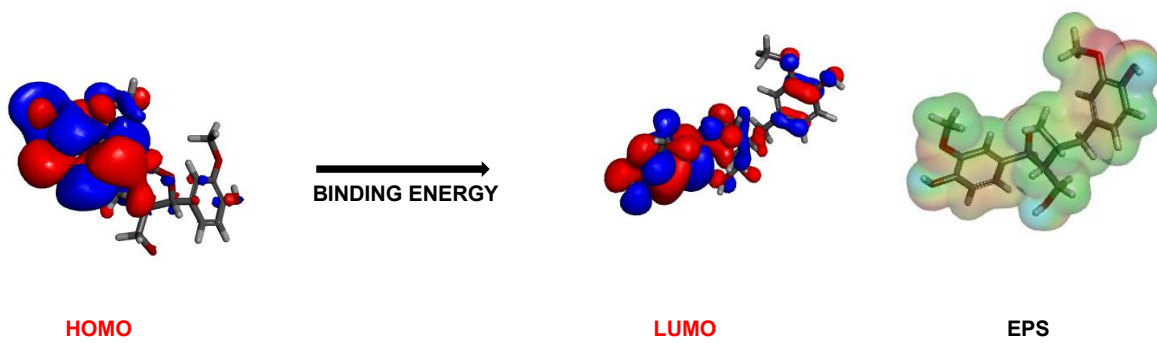


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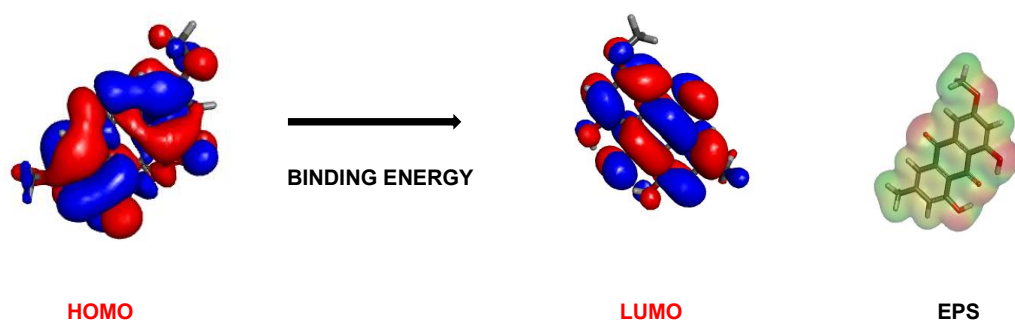
LUMO

EPS

IMPHY003496



IMPHY012117



HOMO AND LUMO:

In the Comprehensive Study of Therapeutic Potential of Indigenous Herbal Plants Against Gynecological Cancer Target-PIK3CA, the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) can be important parameters in understanding the potential anti-cancer activity of the active compounds in the herbal plants.

The HOMO represents the highest energy level of an electron that is occupied by a molecule in its ground state, while the LUMO represents the lowest unoccupied energy level. The energy difference between these orbitals, known as the HOMO-LUMO gap, can provide information about the chemical reactivity of a molecule, including its ability to donate or accept electrons.

The HOMO and LUMO energies of the active compounds can provide insights into their potential interaction with the PIK3CA protein. For example, if the HOMO of an active compound is located near the LUMO of the PIK3CA protein, it could potentially donate electrons to the protein, forming a strong interaction. Additionally, the HOMO-LUMO gap can provide information about the stability and reactivity of the active compounds, and can be used to predict their potential cytotoxicity against cancer cells.

Overall, the HOMO and LUMO energies of the active compounds in the herbal plants can be important parameters to consider in the Comprehensive Study of Therapeutic Potential of Indigenous Herbal Plants Against Gynecological Cancer Target-PIK3CA, as they can provide valuable information about their potential anti-cancer activity and mechanism of action.

ELECTRON DENSITY SURFACE:

EPS (electron density surface) can be a useful tool for visualizing the electrostatic potential of the active compounds in the Comprehensive Study of Therapeutic Potential of Indigenous Herbal Plants Against Gynecological Cancer Target-PIK3CA. EPS can provide a 3D representation of the electron density around a molecule, which can help identify regions of high or low electron density, and therefore, regions of high or low electrostatic potential. In the context of the study, EPS can be used to

visualize the potential binding sites and interactions between the active compounds and the PIK3CA protein.

For example, if the EPS of an active compound shows regions of high electron density, it could indicate the presence of electron-rich functional groups that are capable of interacting with positively charged amino acid residues on the surface of the protein. Furthermore, EPS can be used to identify potential hydrogen bonding interactions between the active compounds and the protein. Hydrogen bonding is a type of electrostatic interaction that occurs between a hydrogen atom bonded to an electronegative atom (such as oxygen or nitrogen) and a nearby electronegative atom. By analyzing the EPS, researchers can identify potential hydrogen bond donors and acceptors in the active compounds and the protein, which can facilitate strong binding interactions.

Overall, EPS can be a valuable tool for understanding the electrostatic interactions between the active compounds in the herbal plants and the PIK3CA protein, and can aid in the development of more effective anti-cancer therapies.

FUTURE SCOPE:

Clinical Trials: The in vitro and in vivo results obtained from this study could provide a basis for the development of clinical trials involving the use of these indigenous herbal plants as an alternative or adjunct treatment for gynecological cancer. Clinical trials could help to validate the efficacy and safety of these herbal plants in humans, and provide additional evidence to support their use in cancer therapy.

Mechanistic Studies: The study focused on the effects of these herbal plants on the PIK3CA pathway. Further mechanistic studies could investigate the underlying molecular mechanisms of action of these plants and how they interact with other pathways and molecules involved in cancer development and progression.

Chemical Characterization: The identification and isolation of active compounds from these indigenous herbal plants could provide important insights into their therapeutic potential against gynecological cancer. Chemical characterization studies could help to identify specific compounds that are responsible for the observed anticancer activity and to optimize their chemical structures for better efficacy and safety.

Combination Therapy: The study investigated the effects of individual herbal plants on the PIK3CA pathway. Future studies could explore the potential of combining these plants with other chemotherapeutic agents or targeted therapies for synergistic effects.

Pharmacokinetic and Pharmacodynamic Studies: Future studies could investigate the pharmacokinetics and pharmacodynamics of these herbal plants in order to better understand their absorption, distribution, metabolism, and excretion, as well as their biological effects on cancer cells and normal tissues.

Overall, the comprehensive study of the therapeutic potential of indigenous herbal plants against gynecological cancer target-PIK3CA has many potential future directions, which could lead to the development of effective and safe herbal treatments for gynecological cancer.

SUMMARY AND CONCLUSION:

Gynecological cancer is a major health issue worldwide, and the PI3K/AKT/mTOR pathway is frequently dysregulated in these types of cancers. Targeting the PIK3CA gene in this pathway has emerged as a potential therapeutic strategy, and there is growing interest in the use of herbal medicines to treat cancer due to their low toxicity and potential efficacy. This literature survey reviewed several studies investigating the anticancer potential of various herbal plants against gynecological cancer cells targeting PIK3CA.

However, more research is needed to fully understand the mechanism of action and potential clinical applications of these herbal plants. Further preclinical and clinical studies are necessary to evaluate their efficacy and safety, as well as their potential for use in combination therapy with other conventional treatments.

Overall, the findings of this literature survey highlight the potential of indigenous herbal plants as a valuable source for the development of new anticancer agents against gynecological cancer target-PIK3CA.

Conclusion:

The PI3K/AKT/mTOR pathway is a potential therapeutic target for gynecological cancer, and herbal plants have shown promise in targeting this pathway. The studies reviewed in this literature survey provide evidence for the antiproliferative and apoptotic effects of herbal plants against gynecological cancer cells. However, more research is needed to fully understand the mechanism of action and potential clinical applications of these herbal plants.

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