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(RESEARCH ARTICLE)

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In Silico molecular docking studies of bioactive compounds from *Costus pictus* for their anticancer potential

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Abstract

The *Costus pictus*, D. Don, is a member of the Costaceae family and is usually referred to as spiral ginger. It is a miracle treatment for diabetes. Its leaves aid in the body's ability to accumulate insulin. The insulin plant (Jose *et. al.,* 2010[1,2]; Modak *et. al.,* 2007) is the common name for it. The American-grown insulin plant is gaining popularity in India due to its therapeutic benefits. The present study involved GC-MS analysis of plant extracts using two different solvents: ethanol and petroleum ether. The ethanol extract yielded 26 compounds, while the petroleum ether extract revealed 24 compounds. From each extract, 4 compounds were selected for molecular docking studies using the target protein 7E75. The binding energies of the ethanol-derived compounds were -1.6, -2.2, -2.5, and -2.3 kcal/mol, respectively. In contrast, the petroleum ether-derived compounds exhibited binding affinities of -2.7, -2.8, -2.4, and -2.9 kcal/mol. These results suggest that the compounds obtained from the petroleum ether extract have comparatively stronger binding affinities than those from the ethanol extract.

Keywords: *Costus pictus*; Molecular Docking; GC-MS; 7E75 Protein

1. Introduction

Naure has been a source of medical compounds for thousands of years. Many modern medications have been obtained from natural sources, often based on their traditional applications [3]. Plants have long been a source of medicine and pharmaceuticals for mankind. Natural products are increasingly valued for their applications as "alternatives" to chronic diseases in both developed and developing countries. Medicinal plants used in traditional medicine are significantly useful and are commonly available in rural regions at a comparably lower cost than modern medicine. It is estimated that 70 to 80% of the world's population relies mostly on traditional healthcare and herbal treatments [4]. *C. pictus*, known for its hypoglycemic effects, has recently garnered interest for its broad-spectrum pharmacological potential, including antioxidant and anticancer activities. Molecular docking provides a powerful in silico approach for investigating the binding efficiency of phytochemicals to target proteins, thereby aiding in drug development.

2. Materials and methods

2.1. Collection of plant material and Preparation of plant extract

Fresh and healthy *C. pictus* leaves were taken from Palakkad (Kerala, India), *C. pictus* leaves were thoroughly cleaned, shade-dried at room temperature, and milled into fine powder. The powdered material is then stored in airtight vials

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for later analysis. The homogenized samples were extracted using ethanol, petroleum ether, and distilled water. 20 g of materials were dissolved separately in three conical flasks containing 150 ml of ethanol, petroleum ether, and distilled water.

Figure 1 A. The study plant – *C. pictus* D. Don, B. *C. pictus* leaves powder

2.2. Analysis of Gas Chromatography-Mass Spectrometry:

The components of the mixture are separated by gas chromatography, and each component is evaluated independently using mass spectroscopy. Chemical investigations indicate that it is mostly composed of volatile and non-volatile compounds. GC-MS analysis can provide valuable insights into the metabolic activity of endophytic bacteria, including the metabolites they produce and the environmental conditions that promote their growth. In GC-MS, the material is evaporated and broken down into its constituent chemical elements using a gas chromatography column. After the separated components have been ionized and processed through it, a mass spectrometer is used to identify and measure the mass and abundance of each.

2.3. Compound Selection

From each extract, four compounds with known and potential anticancer properties were selected for docking studies.

2.4. In Silico studies using GC-MS Compounds:

2.4.1. Molecular Docking:

Molecular docking is a novel, focused strategy that is essential to the development and identification of new drugs. This computer-based drug design method is based on mathematical algorithms that allow for the evaluation of the medication's and target molecule's successful biological binding confirmation. It is possible to model and predict the molecular interactions and biochemical processes under assessment since drug design is based on molecular structure [5].

2.4.2. Preparation of Protein:

The PDB ID and three-dimensional structure of the drug targets were obtained from the https://www.rcsb.org/ website. Complete docking steps and calculations were carried out using AutoDock Vina.

2.4.3. Preparation of Ligand:

Numerous compounds have been found based on the results of GC-MS analysis; a small number of these compounds were chosen. An open-source software program called Open Babel was used to convert the SDF files of the chosen chemicals from the PubChem database to PDB format.

2.4.4. Ligand – Protein Docking:

Ligand-protein docking was carried out in AutoDock Vina, an interactive molecular graphics program for computing that displays workable docking strategies for protein and ligand combinations arranged in a hierarchy based on binding affinities.

2.4.5. Lipinski's Rule of 5 (Ro5):

Pfizer's rule of five, as it is commonly known, is applied when choosing a ligand. This is a general guideline for evaluating drug similarity or determining whether a chemical molecule with a specific biological or therapeutic function possesses both chemical and physical characteristics that could likely make it an oral medicine in humans. Following his discovery that many medications taken orally are very small and lipophilic molecules, Christopher A. Lipinski developed this rule in 1997 [6].

Lipinski's rule states that an orally active medication can have no more than one violation of the following conditions.

- Hydrogen bond donors should not exceed 5
- Hydrogen bond acceptors should not exceed
- Molecular weight must be less than 500 Da
- Octanol-water partition coefficient (Log P) should not exceed 5.
- Molar refractivity must be between 40 – 130.

2.4.6. Properties of Lead Likeness

Swiss ADME is a free tool for producing therapeutic qualities such as drug similarity and physicochemical properties of all chemicals, as well as biological or pharmacological activities. Lipinski's criteria determine whether a chemical compound has certain pharmacological and biological properties.

2.4.7. Toxicity

The toxicity of the chemicals was determined using AdmetSAR, a free web server. This web server provides the chemicals' possible toxicity profile along with values that show safety.

3. Results

The GC-MS analysis of *C. pictus* leaves extract was performed by using Thermo GC-MS Trace Ultra Ver: 5.0, with a split injector and a Thermo MS DSQ by using two solvents, ethanol and petroleum ether.

3.1. In silico studies molecular docking:

3.1.1. Ethanol

Gas Chromatography-Mass Spectrometry (GC-MS) analysis of *C. pictus* leaf extracts was performed using a Thermo GC-MS Trace Ultra Version 5.0 system equipped with a split injector and a Thermo MS DSQ detector. Two solvents, ethanol and petroleum ether, were used for extraction. The GC-MS analysis of the ethanol extract revealed 24 but four major bioactive compounds showed the potential anticancer properties: 1-Dodecene, 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl, Neophytadiene, and Phytol acetate. These compounds were subsequently selected for in silico molecular docking studies. The molecular docking studies targeted the protein 7E75, which contains both pro- and anti-apoptotic domains. This protein regulates mitochondrial integrity and includes killer domains located in a surface groove that inhibit apoptosis. The interaction of the selected compounds with 7E75 was assessed to evaluate their potential role in modulating apoptotic pathways for anticancer applications.

Table 1 Results of docking between the drug targets with Ligand using the software programs iGEMDOCK and AutoDock **Vina.**

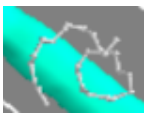
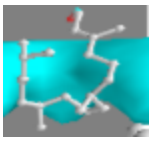
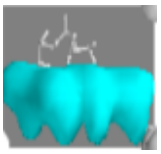
Name of the compound	**Ligand**	**Binding Affinity Kcal/mol**	**rmsd/ub**	**rmsd/lb**	**Binding of protein and ligand**
Pentacosane	7e75_12406_uff_E=6512.60	-1.6	0	0	
2-Pentadecanone, 6,10,14-trimethyl	7e75_10408_uff_E=226.28	-2.2	0	0	
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	7e75_10446_uff_E=225.62	-2.5	0	0	
Neophytadiene	7e75_10446_uff_E=244.25	-2.3	0	0	

Figure 2 PDB Structures of Protein 7E75

When the regulatory ligands are docked with the protein PDB ID 7E75, all the inhibitors' binding sites—that is, amino acid residues—occupy active protein pockets, as shown in Figure 3 (PyMOL).

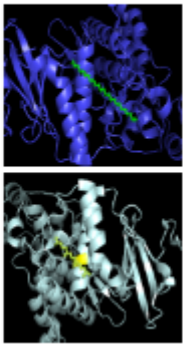
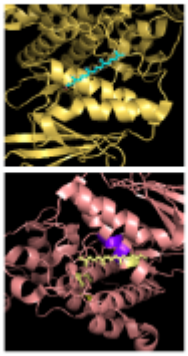
Ligand +protein	3D visual of protein and ligand molecule	Ligand+ protein	3D visual of protein and ligand molecule
Pentacosane 2-Pentadecanone, 6,10,14-trimethyl		3,7,11,15-Tetramethyl-2-hexadecen-1-ol Neophytadiene	

Figure 3 Using Pymol to visualize protein-ligand interactions

Table 2 General properties of (Pentacosane, 2-Pentadecanone, 6,10,14-trimethyl,3,7,11,15-Tetramethyl-2-hexadecen-1-ol, Neophytadiene) such as molecular formula, canonical smiles, and IUPAC name

Name of the Ligand/compound	Chemical formula	SMILES	IUPAC Name
Pentacosane	$C_{25}H_{52}$	CCCCCCCCCCCCCCCCCCCCCCCCC	Pentacosane
2-Pentadecanone, 6,10,14-trimethyl	$C_{18}H_{36}O$	CC(C)CCCC(C)CCCC(C)CCCC(=O)C	6,10,14-trimethylpentadecan-2-one
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	$C_{20}H_{40}O$	CC(C)CCCC(C)CCCC(C)CCC/C(=C/CO)/C	(*E*)-3,7,11,15-tetramethylhexadec-2-en-1-ol
Neophytadiene	$C_{20}H_{38}$	CC(C)CCCC(C)CCCC(C)CCCC(=C) C=C	7,11,15-trimethyl-3-methylidenehexadec-1-ene

Table 3 Physicochemical properties show the number of atoms, molecular weight, fraction CSP3, topological polar surface area, and number of rotatable bonds, molar refractivity. Pentacosane, 2-pentadecanone,6,10,14-trimethyl, 3,7,11,15-tetramethyl-2-hexadecen-1-ol, and Neophytadiene, representing their importance, have good oral bioavailability properties.

Molecules	Molecular Weight (g/mol)	No. heavy atoms	No. atom. heavy atoms	Fraction CSP3	No. rotatable bonds	No. H-bond acceptors	No. H-bond donors	Molar refractivity	TPSA ($^{o}A^{2}$)
1	352.68	25	0	1.00	22	0	0	122	0.00 $Å^2$
2	268.48	19	0	0.94	12	1	0	88.84	17.07 $Å^2$
3	296.53	21	0	0.90	13	1		98.94	20.23 $Å^2$
4	278.52	20	0	0.80	13	0	0	97.31	0.00 $Å^2$

Table 4 Lipophilicity and hydrophilicity of Pentacosane, 2-pentadecanone,6,10,14-trimethyl, 3,7,11,15-tetramethyl-2 hexadecene1-ol, and Neophytadiene

Lipophilicity		**Hydrophilicity**											
Molecules	Consensus Log P	ESOL Log S	ESOL Solubility (mg/ml)	ESOL Solubility (mol/l)	ESOL Class	Ali Log S	Ali Solubility (mg/ml)	Ali Solubility (mol/l)	Ali Class	Silicos-IT LogSw	Silicos-IT Solubility (mg/ml)	Silicos-IT Solubility (mol/l)	Silicos-IT class
1	9.72	-8.87	4.81e-07	1.36e-09	Poorly soluble	-13.21	2.19e-11	6.20e-14	Insoluble	-9.92	4.21e-08	1.19e-10	Poorly soluble
2	5.66	-5.09	2.18e-03	8.11e-06	Moderately soluble	-7.12	2.03e-05	7.56e-08	Poorly Soluble	-5.55	7.50e-04	2.79e-06	moderately soluble
3	6.21	-5.98	3.10e-04	1.05e-06	Moderately soluble	-8.47	9.94e-07	3.35e-09	Poorly soluble	-5.51	9.06e-04	3.05e-06	Moderately soluble
4	7.07	-6.77	4.74e-05	1.70e-07	Poorly soluble	-9.53	8.15e-08	2.93e-10	Poorly soluble	-6.11	2.18e-04	7.82e-07	Poorly soluble

Table. 5 Pharmacokinetics properties of Pentacosane, 2-pentadecanone,6,10,14-trimethyl, 3,7,11,15-tetramethyl-2-hexadecen-1-ol, and Neophytadiene

Molecules	**GI absorption**	**BBB permeant**	**P-gp substrate**	**CYP1A2 inhibitor**	**CYP2C19 inhibitor**	**CYP2C9 inhibitor**	**CYP2D6 inhibitor**	**CYP3A4 inhibitor**	**Log-Kp (cm/s)**
1	Low	No	Yes	No	No	No	No	No	0.89
2	High	No	Yes	No	No	Yes	No	No	-3.00
3	Low	No	Yes	No	No	Yes	No	No	-2.29
4	Low	No	Yes	No	No	Yes	No	No	-1.17

GI absorption: Gastrointestinal absorption, BBB: Blood Brain Barrier, CYP: cytochrome

Table 6 Druglikeness and leadlikeness of Pentacosane, 2-pentadecanone,6,10,14-trimethyl, 3,7,11,15-tetramethyl-2-hexadecen-1-ol, and Neophytadiene

Molecules	**Lipinski #violations**	**Ghose #violations**	**Veber**	**Egan**	**Muegge #violations**	**Bioavailability Score**	**PAINS #alerts**	**Brenk #alerts**	**Leadlikeness #violations**	**Synthetic Accessibility**
1	1	No	No	No	No	0.55	0	0	No	3.32
2	1	No	No	No	No	0.55	0	0	No	3.20
3	1	No	No	No	No	0.55	0	1	No	4.30
4	1	No	No	No	No	0.55	0	1	No	4.08

Table. 7 Tabulates the toxicity profile of the compounds of Pentacosane, 2-pentadecanone,6,10,14-trimethyl, 3,7,11,15-tetramethyl-2-hexadecen-1-ol, and Neophytadiene, which were non-toxic in hERG, AMES toxicity, acute oral toxicity, and Human oral bioavailability

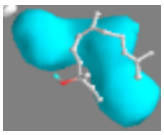
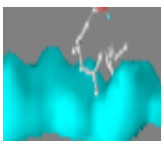
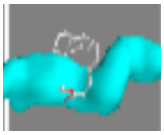
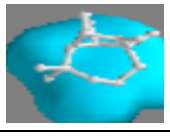
Name of ligand	*hERG* inhibition	AMES toxicity	Carcinogenicity (Class III)	Acute oral toxicity (kg/mol)	Human oral bioavailability
Pentacosane	0.856	0.098	0.33	-3.849	0.237
2-Pentadecanone, 6,10,14-trimethyl	0.709	0.035	0.136	-4.02	0.449
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	0.772	0.041	0.198	-4.047	0.495
Neophytadiene	0.768	0.056	0.199	-3.996	0.471

hERG- human Ether a-go-go related gene

3.1.2. Petroleum ether

The GC-MS analysis of the ethanol extract revealed 26 but four major bioactive compounds showed potential anticancer properties: 1-Dodecene, 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl, Neophytadiene, and Phytol acetate. These compounds were subsequently selected for in silico molecular docking studies. The molecular docking studies targeted the protein 7E75, which contains both pro- and anti-apoptotic domains. This protein regulates mitochondrial integrity and includes killer domains located in a surface groove that inhibit apoptosis. The interaction of the selected compounds with 7E75 was assessed to evaluate their potential role in modulating apoptotic pathways for anticancer applications.

Table 8 Results of docking between the drug targets with Ligand using the software programs iGEMDOCK and AutoDock Vina

Name of the compound	Ligand	Binding Affinity Kcal/mol	rmsd/ub	rmsd/lb	Binding of protein and ligand
d-Nerolidol	7e75_5356544_uff_E=159.25	-2.7	0	0	
Phytol	7e75_5280435_uff_E=225.62	-2.8	0	0	
9-Octadecen-12-ynoic acid, methyl ester	7e75_5363161_uff_E=2126.39	-2.4	0	0	
Junipene	7e75_1796220_uff_E=543.84	-2.9	0	0	

When the regulatory ligands are docked with the protein PDB ID 7E75, all the inhibitors' binding sites—that is, amino acid residues—occupy active protein pockets, as shown in Figure 4 (PyMOL).

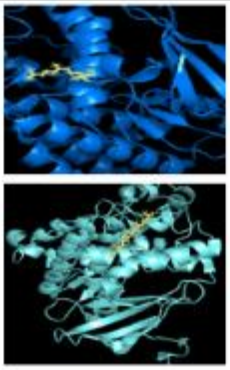
Ligand +protein	3D visual of protein and ligand molecule	Ligand+ protein	3D visual of protein and ligand molecule
d-Nerolidol Phytol		9-Octadecen-12-ynoic acid, methyl ester Junipene	

Figure 4 Using Pymol to visualize protein-ligand interactions

Table 9 General properties of (d-Nerolidol, a-sesquiphellandrene,9-octadecen-12-ynoic acid, methyl ester, Junipene) such as molecular formula, canonical smiles, and IUPAC name

Name of the Ligand/compound	Chemical formula	SMILES	IUPAC Name
d-nerolidol	C15H26O	CC(=CCC/C(=C\CC[C@@] (C)(C=C)O)/C)C	(3S,6Z)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol
Phytol	C20H40O	C[C@@H](CCC[C@@H] (C)CCC/C(=C/CO)/C) CCCC(C)C	(E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-ol
9-octadecen-12-ynoic acid, methyl ester	C19H32O2	CCCCCC#CC/C=C/CCCCCCCC(=O)OC	Methyl(E)-octadec-9-en-12-ynoate
Junipene	C13H20	C=C1[C@H]2CC[C@H]3[C@]1(C)CCCC[C@@H]23	(1R,2S,7S,9S)-3,3,7-trimethyl-8-methylidenetricyclo [5.4.0.02,9] undecane

Table 10 Physicochemical properties show the number of atoms, molecular weight, fraction CSP3, topological polar surface area, and number of rotatable bonds, molar refractivity. D-nerodiol, Phytol, 9-octadecen-12-ynoic acid methyl ester, Junipene, and their importance are represented by their good oral bioavailability properties

Molecules	Molecular Weight (g/mol)	No. heavy atoms	No. atom. heavy atoms	Fraction CSP3	No. rotatable bonds	No. H-bond acceptors	No. H-bond donors	Molar refractivity	TPSA ($^oA^2$)
1	222.37	10	0	0.60	5	0	0	46.61	0.00 $Å^2$
2	83.15	6	0	1.00	3	0	0	27.79	0.00 $Å^2$
3	292.46	21	0	0.74	13	2	0	92.42	26.30 $Å^2$
4	176.30	13	0	0.85	0	0	0	57.53	0.00 $Å^2$

Table 11 Lipophilicity and hydrophilicity of D-nerodiol, Phytol, 9-octadecen-12-ynoic acid methyl ester, Junipene.

Lipophilicity		Hydrophilicity											
Molecules	**Consensus Log P**	**ESOL Log S**	**ESOL Solubility (mg/ml)**	**ESOL Solubility (mol/l)**	**ESOL Class**	**Ali Log S**	**Ali Solubility (mg/ml)**	**Ali Solubility (mol/l)**	**Ali Class**	**Silicos-IT LogSw**	**Silicos-IT Solubility (mg/ml)**	**Silicos-IT Solubility (mol/l)**	**Silicos-IT class**
1	2.80	-2.79	2.18e-01	1.61e-03	soluble	-3.58	3.58e-02	2.65e-04	soluble	-2.42	5.09e-01	3.77e-03	soluble
2	2.26	-2.61	2.02e-01	2.43e-03	soluble	-3.60	2.10e-02	2.52e-04	Soluble	-2.17	5.66e-01	6.81e-03	soluble
3	5.40	-4.90	3.71e-03	1.27e-05	Moderately soluble	-6,86	4.05e-05	1.38e-07	Poorly soluble	-5.37	1.26e-03	4.31e-06	Moderately soluble
4	3.97	-3.72	3.33e-02	1.89e-04	soluble	-4.15	1.25e-02	7.11e-05	moderately soluble	-3.00	1.78e-01	1.01e-03	soluble

Table 12 Pharmacokinetics properties of D-nerodiol, Phytol, 9-octadecen-12-ynoic acid methyl ester, Junipene

Molecules	GI absorption	BBB permeant	P-gp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log-Kp (cm/s)
1	Low	Yes	No	No	No	No	No	No	-4.37
2	Low	No	No	No	No	No	No	No	-4.04
3	High	Yes	No	Yes	No	No	No	No	-3.46
4	Low	Yes	No	No	Yes	Yes	No	No	-4.23

GI absorption: Gastrointestinal absorption, BBB: Blood Brain Barrier, CYP: cytochrome

Table 13 Druglikeness and leadlikeness of D-nerodiol, Phytol, 9-octadecen-12-ynoic acid methyl ester, Junipene.

Molecules	Lipinski #violations	Ghose #violations	Veber	Egan	Muegge #violations	Bioavailability Score	PAINS #alerts	Brenk #alerts	Leadlikeness #violations	Synthetic Accessibility
1	1	No	Yes	Yes	No	0.55	0	1	No	2.84
2	1	No	Yes	Yes	No	0.55	0	0	No	1.00
3	1	Yes	No	Yes	No	0.55	0	2	No	3.95
4	1	Yes	Yes	Yes	No	0.55	0	1	No	3.39

Table 14 Tabulates the toxicity profile of the compounds of D-nerodiol, Phytol, 9-octadecen-12-ynoic acid methyl ester, and Junipene. which were non-toxic in hERG, AMES toxicity, acute oral toxicity, and Human oral bioavailability

Nam-e of ligand	hERG inhibition	AMES toxicity	Carcinogenicity (Class III)	Acute oral toxicity (kg/mol)	Human oral bioavailability
D - nerodiol	0.602	0.086	0.488	-3.602	0.093
Phytol	0.428	0.076	0.422	-3.493	0.287
9-octadecen-12-ynoic acid methyl ester	0.697	0.048	0.051	-3.970	0.013
Junipene	0.936	0.149	0.542	-2.764	0.761

hERG- human Ether a-go-go related gene.

4. Discussion

The GC-MS analysis of *C. pictus* leaves extract was carried out using a Thermo GC-MS Trace Ultra Ver: 5.0 with a split injector and a Thermo MS DSQ with two solvents, ethanol and petroleum ether. The GC-MS analysis revealed 26 compounds in the ethanol extract and 24 compounds in the petroleum ether extract. Among both compounds exhibited notable anticancer properties.

In silico studies molecular docking: A computational molecular docking methodology can be used to overcome the limitations of conventional methods. This method reduces the time by effectively determining and assessing the most likely bioactive molecule among a vast array of chemicals. As the stages of medication development and natural product discovery progress, molecular docking is garnering a lot of attention. It can be used to analyse metabolite libraries for powerful medications and simulate the interaction of a possible ligand with a receptor [7] . GC-MS analysis was used to examine various solvent extracts. The molecular docking results for the investigated substances are shown in Table 1 in decreasing order of least to most active. Docking has the advantage of determining the critical interactions that ligands engage in to attach to the enzyme or receptor binding site, as well as forecasting the binding affinity of protein-ligand complexes [8].

In ethanol, the solvent extract was used for docking analysis. 4 compounds were docked using AutoDock Vina, in which all these compounds showed anticancer activity. The anticancer protein, namely 7E75. Pentacosane, 2-pentadecanone,6,10,14-trimethyl, 3,7,11,15-Tetramethyl-2-hexadecen-1-ol, Neophytadiene. The binding energy of these compounds was shown to be -1.6, -2.2, -2.5, and -2.3 kcal/mol, respectively. The physicochemical properties show the number of atoms, molecular weight fraction CSP3, topological polar surface area, and number of rotatable bonds, molar refractivity representing their importance in good oral bioavailability properties. Lipophilicity and hydrophilicity, pharmacokinetics properties, druglikeness and lead likeness, and toxicity profile of the compounds.

In petroleum ether solvent extract was used for docking analysis, in which 4 compounds have anticancer activity. The binding affinity values such as -2.7, -2.8, -2.4, and -2.9 kcal/mol, respectively, obtained by AutoDock Vina D-nerolidol, phytol, 9-octadecen-12-ynoic acid, methyl ester & Junipene. The physicochemical properties, including the number of atoms, molecular weight fraction, CSP3, topological polar surface area, and number of rotatable bonds, as well as molar refractivity, represent their importance in achieving good oral bioavailability properties. Lipophilicity and hydrophilicity, pharmacokinetics properties, druglikeness & leadlikeness

Ethanol and petroleum ether solvent extracts have anticancer properties. The ligand was docked with the target protein 7E75, a protein-coding gene, using iGEMDOCK and AutoDock Vina. The binding affinities and energy values were discovered. The drug similarity &other characteristics of each docked substance were tested, using the tool PubChem. Canonical names& IUPAC names were investigated; lead &drug similarity demonstrate that all compounds obey Lipinski's law of 5. A software tool called SWISS ADME was used for all these studies. The substances' toxicity profiles included acute sublingual toxicity, AMES toxicity &non-toxicity in hERG. Some of the substances were discovered to be both Carcinogenic & non-carcinogenic in terms of their ability to cause cancer.

5. Conclusion: Ethanol and petroleum ether extracts demonstrated anticancer properties. Ligands derived from these extracts were docked with the target protein 7E75, protein, in the context of cancer, is most likely a reference to the E7 oncoprotein, which is encoded by high-risk strains of human papillomaviruses (HPVs). This viral protein plays a critical

role in the development of HPV-associated cancers, especially cervical cancer, due to its ability to disrupt normal cell cycle regulation and promote uncontrolled cell proliferation a protein-coding gene product, using iGEMDOCK and AutoDock Vina. The docking studies revealed binding affinities and energy values indicative of potential therapeutic activity. Gas Chromatography-Mass Spectrometry (GC-MS) analysis of *C. pictus* leaf extracts was performed using a Thermo GC-MS Trace Ultra Version 5.0 system equipped with a split injector and a Thermo MS DSQ detector. Docking studies were conducted with AutoDock Vina and PyMOL. Autodock Vina is an open-source software package that has been validated and widely used for molecular docking studies of ligand and protein interactions for specificity and drug ability. Software known as SWISS ADME was used in all these investigations. Among the toxicity profiles of the medicines were AMES toxicity, acute sublingual toxicity, and non-toxicity in hERG. Several of the compounds were found to be both carcinogenic and non-carcinogenic in terms of their ability to do so.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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