LEBDA MEDICAL JOURNAL, VOL. 11, NO. 1 (30 APRIL 2026), PP. 27–36.

Lebda Medical Journal; |LMJ|; {Online ISSN:2520-095X}

Lebda Medical Journal Homepage: https://lebmedj.elmergib.edu.ly/index.php/LMJ/en

Received:22.01.2026; Revised:11.03.2026; Accepted:21.04.2026; Published:30.04.2026.

Molecular Docking Analysis of Bioactive Compounds from *Lepidiumsativum* as Potential Breast Cancer Inhibitors Using AutoDockVina

Ashraf Ahmed Ali Abdusalam[a]* Asma Alsonosi Abuzahwa[a], Retaj Emraja Ali[a], Zahia Mohmed Ibrahim[a], Nawal Ebrahim Alkhalil[a], Hadeel Mohamed Raheel[a]

[a] Faculty of health Sciences, Sirte University, Sirte Libya

* Corresponding author email: aalmansory@su.edu.ly

ABSTRACT

Breast cancer is a complicated and multidimensional disease that has emerged as one of the world's top causes of death for w omen, which emphasises the significance of developing novel and efficient treatments. Molecular docking has become an essential part of drug discovery and facilitating the identification of possibilities of therapeutic agents, as it predicts the binding affinities of the therapeutic agents to the target proteins. A molecular docking analysis of 10 bioactive compounds of Lepidium sativum with the target protein of tyrosine kinase (Protein Data Bank (PDB) ID: 1M17) was done using AutoDock Vina to identify potential breast cancer inhibitors. The top 4 compounds identified that displayed high binding affinity to the target breast cancer protein were stigmasterol (-9.6 kcal/mol), 1,3-dibenzyl-1,3-bis[(1R)-1-benzyl-2-hydroxy-ethyl]urea (-8.4 kcal/mol), semilepidinside (-7.7 kcal/mol), and delta-tocopherol (-7.4 kcal/mol). Through detailed analysis of binding poses, the molecular interaction reveals that these compounds exhibited different interactions such as hydrogen bonding and hydrophobic interactions with the essential amino acids in the binding pocket. These results propose the identified phytochemicals in Lepidium sativum as possible potential candidates as breast cancer inhibitors. Nevertheless, additional in vitro and in vivo experiments are required to confirm those computational results and investigate their therapeutic possibilities.

Keywords; Breast cancer, Molecular docking, Lepidiumsativum, drug discovery

1. Introduction

Breast cancer ranks among the most frequently diagnosed cancers globally and is a primary contributor to morbidity and mortality. GLOBOCAN 2020 reported around 2.3 million new cases globally, underscoring its extensive prevalence. It represents a substantial public health challenge across many demographics and constitutes about 25% of all cancer cases in women, rendering it the most often diagnosed cancer among females. (1). The death rates are significantly high, approximately 88% in the areas with socioeconomic transitions (Melanesia, Western Africa, and the Caribbean) rather than the fully developed ones, such as Australia, Western Europe, and Northern America. The early detection and prevention approaches, using screening programmes, are critical to minimising the occurrence of breast cancer and enhancing treatment results. The Breast Health Global Initiative (BHGI) is the organization that spearheads the attempts to formulate international standards in managing breast cancer (2). The rates vary according to geographical area and are higher in the developed countries

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countries, where access to screening programs and healthcare resources is more prevalent. Although breast cancer mostly occurs in women, 1 percent of the cases are in males. The risk of the disease is correlated with the ages: the diagnoses begin to be more common after 50 years old, but younger women and even adolescents can be occasionally diagnosed with the disease. Certain health care interventions will be improved by an understanding of these epidemiological trends (3). Breast cancer risk factors can be divided into non-modifiable (e.g., genetic mutation: BRCA1, BRCA2), gender, age, and personal cancer history; and modifiable (e.g., obesity, alcohol, and hormone replacement therapy (HRT)). These risk factors are identified, which helps in the effective prevention and risk assessment. Several molecular subtypes of breast cancer that are different in their profile include hormone receptor-positive (HR+), epidermal growth factor receptor tyrosine kinase domain (EGFR TKD), and triple-negative breast cancer (TNBC). Each subtype informs specific treatment strategies and has varying prognostic outcomes (4,5) which means that understanding these differences is crucial for tailoring individualised treatment plans for patients with breast cancer. *Lepidiumsativum* (garden cress) is an annual herb that belongs to the *Brassicaceae* family and is known to have medicinal effects, particularly in areas such as South Asia. Garden cress has traditionally been used in the management of various conditions, including bronchitis, asthma, and rheumatism, and is similarly valued as a diuretic, digestive aid, and mild laxative due to its high content of phytochemicals such as alkaloids, glucosinolates, and flavonoids (6). In India, Cassia cress seeds, leaves, and roots are similarly utilized in the management of health conditions, where they serve as anti-inflammatory agents, galactagogues, and blood purifiers (7). *Lepidiumsativum* has demonstrated anticancer, antimicrobial, antioxidant, anti-asthmatic and diuretic effects. Research has shown that it has potential in causing cancer cell apoptosis and combating bacterial infections, in addition to eliminating free radical scavenging (8–10). Molecular docking is an important tool in drug discovery that allows the interaction between the ligand and the receptor to be simulated in predicting the binding affinities and drugs working mechanisms. Recent developments such as reverse molecular docking give more insights into drug-target interactions that can prove to be more efficient in undertaking pharmacological evaluations (11,12). AutoDockVina (13) is the latest update version of a molecular docking and virtual screening application, with reliable precision in predicting ligand–receptor interactions. AutoDockVina is significantly faster than its predecessor, AutoDock 4, with reported speed improvements of up to two orders of magnitude (approximately 100-fold), depending on the system and computational settings. AutoDockVina is more precise when predicting binding modes, as confirmed by the training set on which it was tested first on AutoDock 4. It uses multi-core systems to use Multithreading capabilities to increase speed. AutoDockVina makes the user experience easier by taking care of grid map computations and sorting its results automatically (14, 15). The study aims to utilize *in silico* molecular docking techniques and apply them to identify and evaluate potential inhibitors obtained from the *Lepidium sativum* plant against EGFR TKD, followed by interaction analysis to identify promising lead compounds for breast cancer therapy.

2. Materials and Methods

2.1 Protein preparation

The three-dimensional crystal structure of the Epidermal Growth Factor Receptor tyrosine kinase domain (EGFR TKD) (PDB ID: 1M17) (16) was retrieved from the RCSB Protein Data Bank . The protein structure was prepared using AutoDockTools (ADT) (ADT) (17) as shown in Figure 1. The protein structure was prepared using AutoDockTools (ADT) v1.5.6. All non-essential water molecules and co-crystallized ligands were removed. Polar hydrogen atoms were added, and Gasteiger charges were computed. The prepared protein structure was saved in the PDBQT format for subsequent docking analysis. Chain B was selected for this study.

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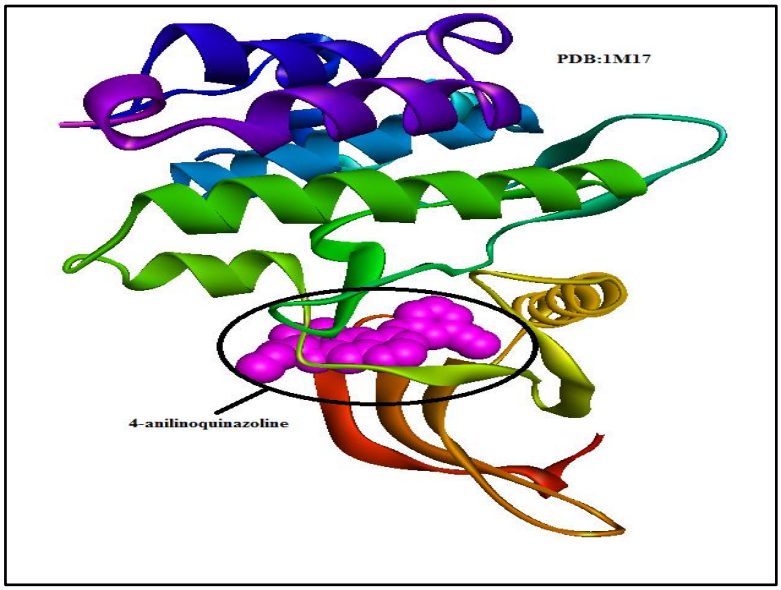

Figure 1. Represent the 3D structure of the tyrosine kinase (Protein Data Bank (PDB) ID: 1M17)

2.2 Ligand preparation

The 2D structures of ten bioactive compounds previously identified in *Lepidium sativum*were obtained from the PubChem database. The structures were converted to 3D format, and their energies were minimized using appropriate computational chemistry tools. The prepared ligands were then saved in PDBQT format, with rotatable bonds defined to allow conformational flexibility during docking.

Ten bioactive compounds were identified in *Lepidium sativum* and their 3D structures were from the PubChem (18) database in SDF format and then converted to PDB to be used in molecular docking using Discovery studio visualiser . The energy was minimised using Avogadro software, and the rotatable bonds are defined to allow conformational flexibility during docking.

2.3 Molecular docking and Grid Generation

Molecular docking simulations were performed using AutoDockVina v1.2.3. A grid box was defined to encompass the active site of the 1M17 protein, ensuring that the ligand search space was centred on the known binding pocket. The grid box was set with dimensions of 22.5 × 22.5 × 22.5 Å and centred at coordinates x = -23.368, y = 29.808, and z = 7.596. Vina's search algorithm explored various ligand conformations, and the pose with the lowest free energy of binding (FEB) was selected as the most probable binding mode.

2.4. Docking Protocol Validation

To validate the accuracy and reliability of the docking protocol, the co-crystallized ligand (4-anilinoquinazoline) was extracted from the complex (PDB) ID: 1M17) and re-docked into the protein's active site. The root-mean-square deviation (RMSD) between the predicted pose and the original crystallographic pose was calculated. An RMSD value below 2.0 Å is generally considered an indicator of a successful and

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reliable docking protocol.

2.5. Drug-Likeness Analysis

The top-ranked compounds were evaluated for their drug-like properties based on Lipinski's Rule of Five. This rule assesses physicochemical properties critical for oral bioavailability, including molecular weight (MW < 500 g/mol), logarithm of the partition coefficient (xLogP< 5), number of hydrogen bond donors (HBD < 5), and number of hydrogen bond acceptors (HBA < 10).

3. Results and Discussion

3.1 Validation of docking procedure

Before conducting molecular docking, we validated the docking protocol by re-docking the co-crystallized 4-anilinoquinazoline into the active site of the target protein (Protein Data Bank (PDB) ID: 1M17) within an acceptable range. In this validation, the pose of the 4-anilinoquinazoline exhibited a similar orientation to the crystallographic pose (RMSD = 0.82 Å), and the binding affinity was -7.2 kcal/mol. Consequently, these results affirm the reliability of the protocol employed, indicating that the docking software can be trusted to accurately reproduce the anticipated binding mode of the co-crystallized ligand as shown in Figure 2.

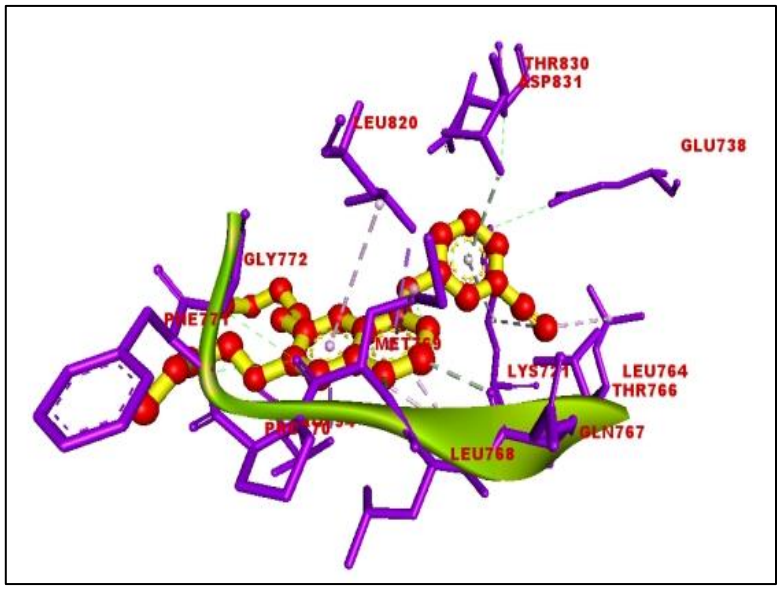

Figure 2. The Superimposition between the docked conformation (yellow) and the crystal structure (Red) in the binding pocket of 1M17 protein.

3.2 Molecular Docking of *Lepidiumsativum* Bioactive Compounds

In the initial phase, we gathered a set of 10 compounds from *Lepidium sativum*, as documented in the literature (19,20)as shown in Table 1. Molecular docking using AutoDock Vina was conducted of these compounds against the target protein, and their arrangement was based on the free energy of binding (FEB). Subsequently, we selected the top four compounds that displayed the lowest binding energy.

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Table 1. Name and structure of ten selected compounds from *Lepidiumsativum* plant

NO	Compounds	AutoDock 4.2 (kcal/mol)
1	stigmasterol	-9.6
2	1,3-dibenzyl-1,3-bis[(1R)-1-benzyl-2-hydroxy-ethyl]urea	-8.4
3	Semilepidinoside A	-7.7
4	Delta tochpherol	-7.4
5	Butylatedhydroxytoluene	-6.9
6	methyl glucosinolate	-6.1
7	Oleic acid	-5.3
8	Eicosenoic acid	-5.2
9	Benzyl cyanide	-5.0
10	Arachidic acid	-4.8

3.3 Free Energy of Binding and Ranking of Docked Compounds

As shown in Figure 3, the 2D structure of the top four bioactive compounds ranked by AutoDockVina scores, these molecules exhibited the lowest FEB among the other compounds in the protein-ligand complex; subsequently, they were applied in the docking calculation. The docking simulation results showed that all the 20 compounds displayed FEB in the range -9.6 to -4.8 kcal/mol. Therefore, the compounds that showed the lowest FEB were considered the best, as shown in Table 2. Therefore, the top 4 ranked compounds were suggested as the most suitable candidates. Stigmasterol,1,3-dibenzyl-1,3-bis[(1R)-1-benzyl-2-hydroxy-ethyl]urea , semilepidinside and Delta-tochpherol displayed a minimum FEB of -9.6, -8.4, and -7.7 and 7.4 kcal/mol by AutoDockVina.

Table 2. Molecular properties of the 5 compounds obtained from Lepidiumsativum plant

NO	Compounds	xlogP	H-bond donors	H-bond acceptors	MW(g/mol)	Rotatable bonds
1	stigmasterol	8.32	1	1	420.45	6
2	1,3-dibenzyl-1,3-bis[(1R)-1-benzyl-2-hydroxy-ethyl]urea	5.40	2	3	508.65	14
3	Semilepidinoside A	-0.43	5	7	336.34	5
4	Delta tochpherol	9.97	2	1	402.65	12

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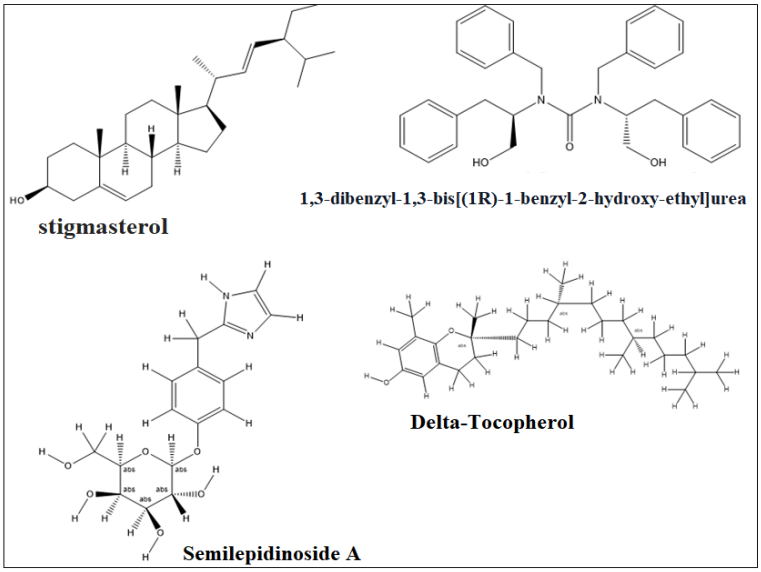

Figure 3. four compounds from *Lepidiumsativum*Stigmasterol , 1,3-dibenzyl-1,3-bis[(1R)-1-benzyl-2-hydroxy-ethyl]urea, Semilepidinoside A and Delta tochpherol.

3.4 Drug Likeness and Lipinski's Rule of Five Analysis

To further assess their drug-likeness properties, we applied Lipinski's Rule of Five (21), which considers specific molecular properties in comparison to approved drugs. This rule dictates that potential drug candidates should not exceed one violation of the following criteria: ALogP< 5, molecular weight < 500, number of hydrogen bond donors (HBD) < 5, number of hydrogen bond acceptors (HBA) < 10, and rotatable bonds < 10. Notably, all three selected compounds show some violation from the acceptable range defined by the Lipinski rule, as shown in Table 2. This rule is used to determine the drug-likeness properties should be no more than one violation of the following criteria: xLogP< 5, molecular weight < 500, number of HBD < 5, number of HBA < 10, and rotatable bond < 10. As can be seen from Table 2, the three compounds fall within the acceptable range of the Lipinski rule; the stigmasterol compound violates only one rule, 1,3-dibenzyl-1,3-bis[(1R)-1-benzyl-2-hydroxy-ethyl]urea compounds violates the rule of 5 in three rules, semilepidinside compound was ompounds violate the rule of 5 , Delta-tochpherol compound violates two rules.

3.5 Molecular Interaction Analysis of Top Ranked Compounds

3.5.1 Interaction Profile of Stigmasterol

The compound stigmasterol exhibited various interactions as follows: Five hydrogen bonds were formed, with four of them involving amino acids Ser144, Cys145, Gly143, Leu141, and the oxygen atom O2. The fifth hydrogen bond was established between Arg188 and another oxygen atom (O_2) on the compound. Three Pi-Alkyl bonds were observed, with amino acids His41, Cys145, and Pro168 forming bonds with the benzene ring and methyl group, respectively. A Pi-Sulphur bond was exhibited by His163 with a benzene ring on the compound.

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Hydrophobic interactions occurred with amino acids Thr190, Pro168, Gln189, Glu166, Arg188, Met165, Asn142, and His41 at the binding pocket. Van der Waals interactions were noticed between Thr190, Gln192, Glu166, and Asn142, and the carbon atoms C-1, C-5, C-11, and C-14 of the compound. A carbon-hydrogen bond was formed between the amino acid Gln189 and the benzene ring as shown in Figure 4,5, Table 3).

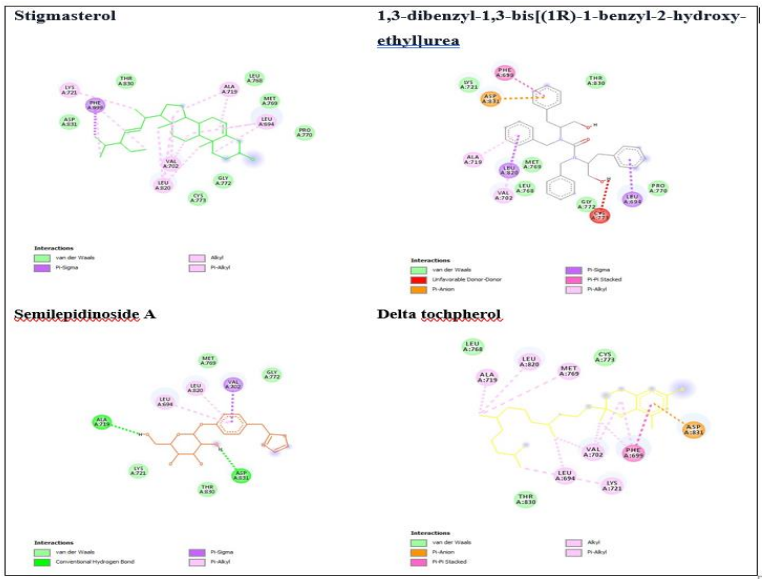

Figure 4. 2D of Binding modes of the selected compounds at breast cancer binding site.

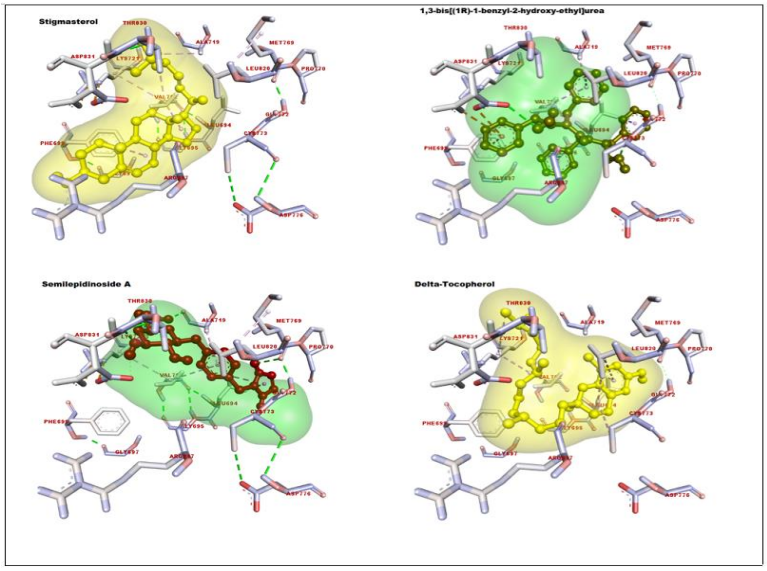

Figure 5. 3D of Binding modes of the selected compounds at breast cancer binding site

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Table 3. Binding interactions details of the Potential ten compounds docked into active site

No	Ligands	AutoDockVina (kcal/mol)	Residue	Type of interactions
1	Stigmasterol	-9.6	Cys773, Gly772, Pro770,Met769, Leu768, Thr830, Asp831	Van der waals
			Phe699	Pi-Sigma
			Leu820 , Val207 , Leu649	Alkyl
			Ala719 , Lys721	Pi-Alkyl
2	1,3-dibenzy	-8.4	Leu768 , Gly772 , pro770 , Thr830 Lys721	Van der waals
			Leu694 , Leu820	Pi-sigma
			Ala719 , Val702	Pi-Alkyl
			Phe699	Pi-Pi stacked
			Asp831	Pi-anion
			Cys773	Unfavorable donerdoner
3	Semilepidinside	-7.7	Ala719 , Asp831	Conventional Hydrogen bond
			Lys721 , Thr830 , Gly772 , Met769	Van der waals
			Val702	Pi-sigma
			Leu820 , Leu694	Pi-Alkhyl
4	Delta-tocopherol	-7.4	Leu694 , Lys721 , Val702	Alkhyl
			Thr830 , cys773 , Leu768	Van der waals
			Asp831	Pi- anion
			Phe699,	Pi-pi stacked
			Met769, Leu694 , Ala719	Pi-alkhyl

3.5.2 Interaction Profile of 1,3 Dibenzyl 1,3 Bis[(1R) 1 Benzyl 2 Hydroxy Ethyl]urea

The compound 1,3-dibenzyl-1,3-bis[(1R)-1-benzyl-2-hydroxy-ethyl]urea was found to exhibit the following interactions: Van der Waals interactions with the amino acids Leu768, Gly772, Pro770, Thr830, Lys721, and Asp831. Pi-sigma bonds formed interactions between the benzene ring and Leu694 and Leu820. Alkyl and Pi-Alkyl bonds interacting with Ala719 and Val702. Pi-Pi stacking interactions observed between the benzene ring and Phe699. Pi-anion interactions involving the benzene ring and Asp831. Unfavourable donor-donor bonds between the amino acid Cys773 and the alcohol group are shown in Figure 4,5, Table 3).

3.5.3 Interaction Profile of Semilepidinside

The compound Semilepidinside displayed the following interactions: Conventional Hydrogen bond interactions between the alcohol group and Ala719 and Asp831. Van der Waals interactions with the amino acids Lys721, Thr830, Gly772, Met769. Pi-sigma interactions between the benzene ring and Val702. Pi-Alkyl bonds are formed with the benzene ring and Leu820, Leu694 as shown in (Figure 4,5, Table 3).

3.5.4 Interaction Profile of Delta Tocopherol

Additionally, the compound delta-tocopherol demonstrated the following interactions: alkyl and Pi-Alkyl bonds formed with Leu694, Lys721, Val702, Met769, Leu694, and Ala719. Pi-anion interactions between the benzene ring and Asp831. Pi-pi stacking interactions

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observed between the benzene ring and the amino acids Phe699. Van der Waals interactions also formed with the amino acids Thr830, Cys773, and Leu768.

3.6 Implications of Molecular Docking in Natural Product Based Drug Discovery

Molecular docking is considered one of the recent procedures used in drug discovery among numerous sources, especially natural products like medicinal plants. It has been shown to have a major role in the discovery of possible therapeutic agents against different diseases as demonstrated in numerous studies. Molecular docking was used in this research to evaluate bioactive compounds in Lepidium sativum as potential breast cancer target inhibitors. The objective of this work aims at discovering promising compounds that have a high binding affinity to the target protein. The results obtained suggest that the applied methodology is consistent with the study objective.

4. Conclusion

In the current study, molecular docking and molecular interaction analysis were effectively used in search of potential inhibitors of the 1M17 protein, a key target in breast cancer treatment. The four compounds of stegmasterol, 1,3-dibenzyl-1,3-bis[(1R)-1-benzyl-2-hydroxy-ethyllurea, semilepidinside, and delta-tocopherol were found to have high affinity with the 1M17 binding pocket. Free energy of binding (FEB) was heir strong binding affinity (-9.6, -8.4, -7.7, and -7.4 kcal/mol). The selected compounds exhibited different positive interactions, such as hydrogen bonds, hydrophobic and pi-connected interactions, and van der Waals forces with the key amino acid residues at the binding pocket. The most promising docking hits had gone past the Lipinski rule of five and probably become oral active drug. Molecular docking could be used to drastically reduce the cost of the drug synthesis and production. Some of the ingredients of *Lepidium sativum* have the potential to be used as a cancer inhibitor at the molecular level of breast cancer. The significance of this finding is that it underscores the importance of utilizing molecular docking as an initial tool in identifying drugs derived from natural product. The compounds can thus only undergo further in vitro and *in vivo* studies to confirm anticancer activity, safety and pharmacokinetic behaviour before being considered potential therapeutic agents.

ETHICAL STATEMENT:

This research has been done completely through computational methods and publicly accessible data. The software tools that are in use are all freely accessible to use with academic and non-commercial purposes. In this work did not involve human or animal subjects hence no ethical approval was needed.

CONFLICT OF INTEREST

The authors declare that they have no competing interests.

AUTHORS' CONTRIBUTIONS

A.A.A.A. conceived and designed the study, supervised, extracted and analyzed the data, and finalized the manuscript. A.A.A., R.E.A., Z.M.I., N.E.A., and H.M.R. conducted the molecular docking experiments and wrote the initial draft of the manuscript. All authors read and approved the final manuscript.

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Corresponding author email: aalmansory@su.edu.ly