IJPSR (2023), Volume 14, Issue 6 **(Research Article)**

INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES AND RESEARCH

Received on 10 September 2022; received in revised form, 19 October 2022; accepted 17 November 2022; published 01 June 2023

IDENTIFICATION AND VALIDATION OF PALUSTRIC ACID AND ANDROGRAPHOLIDE FROM *OCIMUM BASILICUM* LEAF AS A PROMISING BREAST CANCER INHIBITOR: AN *IN-VITRO* AND *IN-SILICO* ANALYSIS

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Keywords:

Breast cancer, Palustric acid and Andrographolide, Inhibitor, Molecular simulation, Docking studies, MCF-7 cell line

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ABSTRACT: This study aimed at identifying promising breast cancer inhibitors through *in-vitro* and *in-silico* studies. *Ocimum basilicum*. L is a traditional herb used for varied ailments. The present study is designed to evaluate the anti-carcinogenic potency of Palustric acid and Andrographolide against the MCF-7 cell line by *in-vitro* analysis. Further *in-silico* examination was performed to detect and formulate Receptor-ligand complex of estrogen using molecular docking technique. *In-vitro* study was conducted using MTT assay and microscopic examinations to determine the cell viability and morphological changes in MCF-7 cells. *In-silico*, scrutiny was performed using virtual screening, Docking, ADME, and molecular dynamic simulation to evaluate the stability of the compounds. Palustric acid and Andrographolide against the MCF-7 cell line by *in-vitro* analysis. Further *in-silico* examination was performed and showed an outstanding anti-cancer potential, with dose- and time-dependent patterns in MTT assay and through the fluctuating organization of MCF-7 cells. *In-silico* analysis showed that the selected lead compound-complex exhibited good stability and was a highly potent inhibitor against the target breast cancer receptor. This study confirmed that Palustric acid and Andrographolide might be an alternate potential inhibitor against breast cancer.

INTRODUCTION: Breast cancer stays a significant disease and is threatening human being's day-to-day life. The frequency is increasing in most nations and is projected to rise further throughout the following 20 years regardless of current endeavors to forestall sickness [1-3]. The expanded frequency isn't is business as usual since there has been, in most nations, an expansion in quantities of ladies with significant breast disease risk factors, including lower time of menarche, late time of first pregnancy, fewer pregnancies, more limited or no periods of breastfeeding, and later menopause. Other gamble factors which add to the weight of breast malignant growth are the expansion in stoutness, liquor utilization, idleness, and chemical substitution treatment (HRT) [4]. One of the primary drivers of breast malignant growth is the estrogen receptor. Over-articulation of estrogen receptors is found in a number of instances of breast malignant growth. The old-style estrogen pathway immediately restricts estrogen-responsive components by utilizing ligand-actuated ER to adjust quality articulation.

Estrogen may likewise go about as a co-activator of other record components to show oncogenes in bosom most malignant growths in the non-old style pathway [5-7]. Estrogen is one of the five steroidal chemicals, typically the female regenerative chemical [8].

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DOI: 10.13040/IJPSR.0975-8232.14(6).2899-06

This article can be accessed online on www.ijpsr.com

DOI link: http://doi.org/10.13040/IJPSR.0975-8232.14(6).2899-06

Without a doubt, even before the body spends the chemical estrogen, it needs to bind to the proteins called estrogen receptors. Malignant dangerous developments tend to be sensitive to the chemical estrogen, which will work on advancing cancer [9]. The cancer-causing cells have the estrogen receptor on their surface areas, called estrogen receptor-positive threatening development or ER-positive infection. Breast malignancy development is an infection that starts in the tissues of the breast, generally from the inward covering of the lobules or the milk pipes which supply milk [10]. The harmful development related to the channels is called ductal carcinoma, while the illness related to the lobules is called lobular carcinoma [11].

Molecular docking approaches are of marvelous significance in making arrangements and format new medications. This system's objective is to anticipate the exploratory restricting mode and liking of a little particle inside the limiting site of the receptor focus of interest. An effective docking strategy should have the option to accurately anticipate the local ligand representing the receptor restricting site and the related physical-substance Molecular associations [12].

O. basilicum Linn. A plant that finishes its lifecycle within one year and is discovered wild in the tropical, subtropical, and mild areas of the world particularly Ceylon, hot West Asia, Africa, Malayan and Pacific Islands. It has begun in Punjab and is additionally broadly dispersed in tropical and mild districts of India and Pakistan [13]. A wide scope of normally happening compounds has been read broadly for their tremendous potential in the anticipation of malignant growth in the course of the most recent couple of many years.

Phytoconstituents are metabolites found exclusively in *O. basilicum* in exploratory frameworks, which give insurance against different ecological and ingested cancer-causing agents by inciting our cell reinforcement catalysts, advancing DNA fix pathways, and in this way straightforwardly affecting the movement of disease and metastasis. Chemotherapy is one of the therapy procedures utilized wherein normal or engineered drugs are regulated to dial back or defer the different advances associated with metastasis, which incorporates inception, advancement, and movement of disease. Normal reasons for the greater part of the tumors that happen today are the climate and way of life factors. It has been recommended that the essential and main driver of a large portion of the diseases is related to acquired hereditary variations (5%-10%) and obtained hereditary irregularity (90%-95%) brought about by different exogenous as well as endogenous natural specialists [14]. *In-silico*, the technique is an unobtrusive strategy that condenses the time spent testing drug sufficiency.

Our aim of the work on the Identify bioactive mixtures present in *Ocimum basilicum* aqueous leaf extract through gas chromatography-mass spectrometry (GC-MS) investigation and to evaluate the expected bioactive mixtures for malignant disease by Autodock vina and iGEMDOCK against estrogen receptor. Pharmacodynamics and toxicity analysis shows a Palustric acid and Andrographolide are promising drugs for hormone-dependent breast cancer.

MATERIALS AND METHODS:

Plant Collection and Identification: New leaves of *O. basilicum* were accumulated from the Palakarai Zone, Tiruchirappalli, Tamil Nadu, India and submitted to the herbarium sheet of plant material at the Department of Botany, St. Joseph's College, Tiruchirappalli. The leaves were then disguised and dried for around fourteen days. The dried leaves were powdered and taken for further analysis.

Preparation of Extracts: Soxhlet extraction of the plant materials was completed with fluid solvents. 50 grams of the powdered plant material was pressed in Whatman No.1 channel paper and were removed independently with 300 ml of the distilled water for 48 hours. The concentrates were then aggregated at room temperature and put away at 40ºC for additional utilization.

GC-MS Analysis: The Phytochemical examination of aqueous concentrates of *Ocimum basilicum* was exhibited in GC-MS gear. The examination was acted in SHIMADZU/QP2020. Then, at that point, the outcomes were looked at by utilizing the National Institute of Standards and Technology Mass Spectral data set (NIST-MS, 1998) library [15].

Preparation of Receptor: The three-dimensional (3D) structures of drug targets selected in this study were available in PDB database accession No.1X7R but the complete sequence and structure are not available in the PDB; therefore, their 3D structures were obtained by homology modelling. The receptor was obtained from PDB dataset. The homology modeling was performed using MODELLER software (Version: 9.0) using easy modeller as the graphical user [16]. The 3D structure was generated. The generated 3D structure of the model receptor was validated using Ramachandran plot and the SAVES online server tool.

Preparation of Ligand: The compounds are selected were retrieved from PubChem databases. Then ligands are prepared by the SDF files were converted into PDB file format using open babel software.

iGEMDOCK: iGEMDOCK is a set-up of computerized docking/screening instruments [17]. The interface of iGEMDOCK has two primary labels, a docking/screening tag and a post-examining tag. The docking/screening tag is intended to anticipate how compound atoms tie to a receptor of realized 3D design. The anticipated protein-ligand postures can also be performed post-investigated in the post-breaking down tag. This can help, for instance, to direct organic analysts to investigate better folios.

Autodock Vina: AutoDock Vina is another age of docking programming from the molecular graphics lab. It accomplishes huge upgrades in the normal exactness of the limiting mode forecasts, while likewise being up to two significant degrees quicker than AutoDock 4.1 Since the scoring capacities utilized via AutoDock 4 and AutoDock Vina are extraordinary and vague, on some random issue, either program may give a superior outcome.

Pharmacokinetics: Pharmacokinetics portrays and evaluates the progressions on the medication made by the body, incorporates moves and substance change of the particle.

Pharmacodynamics: Pharmacodynamics depicts and quantifies the animal's response when taking the drug, at the clinical, biochemical or sub-nuclear level.

Molecular Dynamics Simulation Studies: To study the protein ligand complex stability, a 100 ns simulation was performed. The MD simulation was performed using GROMACS 2020 [18]. The GROMOS 53a6 force field [19] was employed. A system for the protein-ligand was built by packing the complex in a cubic box (sides a=2 nm, b=2 nm,c=2 nm). The system was neutralized using Na^+ ions. Using the steepest descent algorithm, the solvated system was later put through energy minimization. After the protein complex was minimized, molecular dynamics was performed on the equilibrated solvent and ions around the protein. 100 ps NVT and NPT equilibration was carried out and the resulting temperature, pressure and density values were computed using the in-built gromacs function energy.

With the completion of the equilibration phase, MD was performed for the time duration of 100 ns. At the end of MD, the stability and system energies of the complex were evaluated using root mean square deviation (RMSD), root mean square fluctuations (RMSF), radius of gyration (R_g), and protein-ligand interactions.

RESULTS:

Gas Chromatography-Mass Spectrometry: Gas chromatography-mass spectrometry investigation **Fig. 1** portrays the different mixtures present in the leaves of *Ocimum basilicum*. The chromatogram uncovered the presence of 45 compounds in the explored polyherbal arrangement. The two mixtures, to be specific Palustric acid and Andrographolide, were chosen for analysis based on the Rule of Five, and Retention times are 33.21 and 32.05.

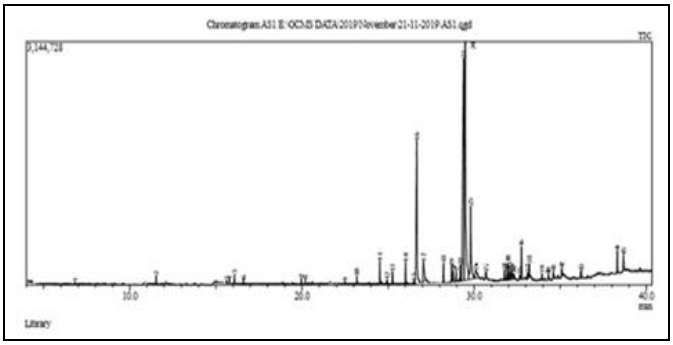

FIG. 1: GAS CHROMATOGRAPHY MASS SPECTROMETRY ANALYSIS OF *OCIMUM BASILICUM*

Homology Modeling: The 3D structures obtained by homology modeling were validated with the aid of the Ramachandran plot as shown in **Fig. 2**.

The Ramachandran plot demonstrated that most of the residues clustered tightly in the most-favored regions with very few outliers for all the drug targets. The Ramachandran plot discovered by G.N. Ramachandran, C. Ramakrishnan and V. Sasisekharan is a way to visualize the dihedral angle, namely Ψ (psi) and φ (phi), of the protein backbone. The receptor estrogen PDB ID: 1x7r contained amino acid residues in the favored region at 97.1%, 2.5% in the allowed region, and 0.4% in the outer region.

They further validated the receptor using the SAVES server. The Ramachandran plot shows the improved acceptability of the overall structures, whereas the point focuses on inside and outside allowed regions and addresses the hard-sphere and cross-over.

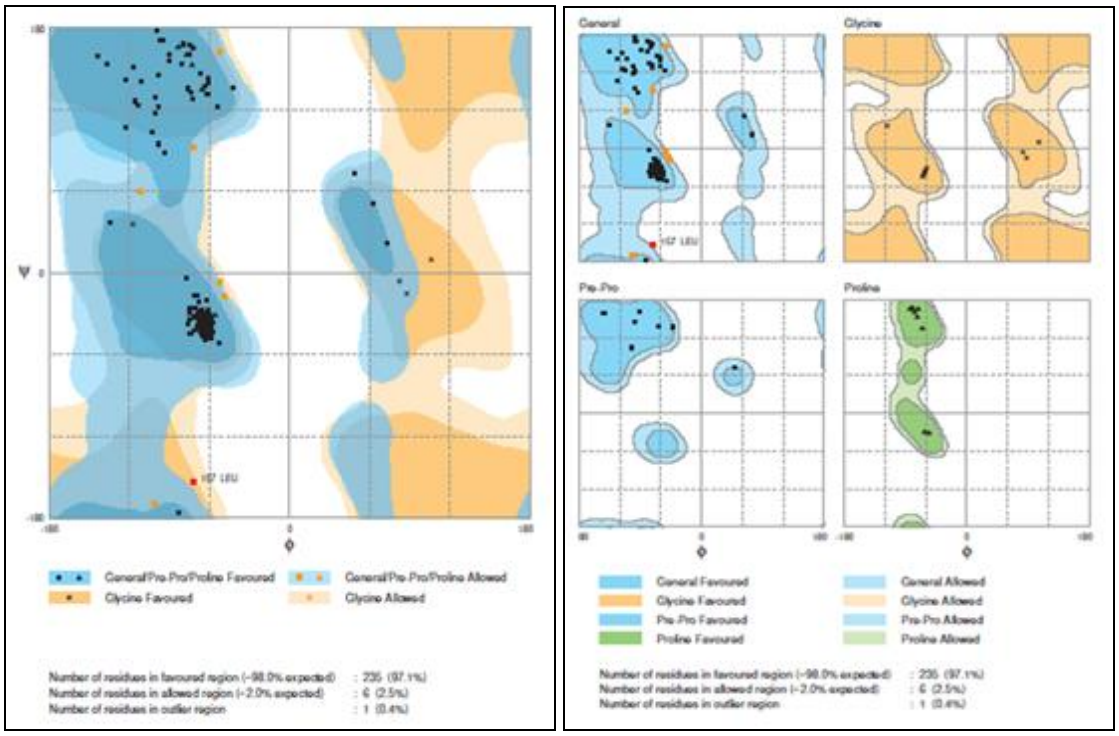

FIG. 2: HOMOLOGY MODELLING

Molecular Docking: *In-silico* devices and *in-vitro* (or *in-vivo*) strategies can be applied synergistically for the fruitful investigation of the inhibitory viability of a compound on a receptor.

Common mixtures have been accounted for to show anticancer properties despite the fact that their activity instrument remains ambiguous. With an end goal to clarify the conceivable catalyst/receptor protein anticarcinogenic communication components hypothetical docking contemplates have been conveyed towards estrogen receptor.

It is one of the steroid hormones naturally present in human reproductive hormones. It can cause tumors in human beings; the selected compounds were docked with iGEMDOCK and Autodock Vina then the structure was viewed in VINA plugin of pymol software, and with the help of grid, the ATP binding site was created. It also narrows the selected compounds based on the binding energy.

Rough Docking Energy Value with Igemdock: IGEMDOCK for *O. basilicum* the objective receptor, in particular estrogen, was docked with palustric acid, andrographolide by iGEMDOCK. **Table 1** shows iGEMDOCK harsh docking results with chosen compounds. The energy esteems are introduced in the table.

The energy esteems the medication got by iGEMDOCK focuses on estrogen receptors alongside palustric acid andrographolide, were -79.23,- 79, Kcal/mol, individually.

TABLE 1: IGEMDOCK ROUGHDOCKING RESULTS WITH SELECTED COMPOUNDS

Drug targets or protein with ligand	Total Energy (Kcal/mol)	VDW (Kcal/mol)	Hbond (Kcal/mol)	Electrostatic (Kcal/mol)	AverConPair (Kcal/mol)
Palustric acid	-79.2305	-77.6932	-1.5374	0	29.5909
Andrographolide	-78.8979	-68.6881	-10.21	0	28

Autodock Vina for *Ocimum basilicum:* The objective Receptor to be specifically estrogen was docked with Palustric acid and Andrographolide *via* Autodock Vina. The Binding energy is introduced in **Table 2**. The Binding energy esteems got *via* Autodock Vina of the medication focuses on Estrogen receptors alongside Palustric acid, Andrographolide, were - 8.95,- 8.91, individually. The docking posture of the mixtures with different medication targets were examined with LigPlot+ programming apparatus. **Fig. 3-4** shows the docking posture of Estrogen receptors alongside Palustric acid, Andrographolide, The docking presents were examined, and the amino acid buildups engaged with the different associations were assessed.

TABLE 2: BINDING AFFINITY WITH AUTODOCK VINA OF SELECTED COMPOUNDS

Ligand	Binding energy	Ranking(For which could be potentially used as a drug)
Palustric acid	-8.95	1
Andrographolide	-8.91	2

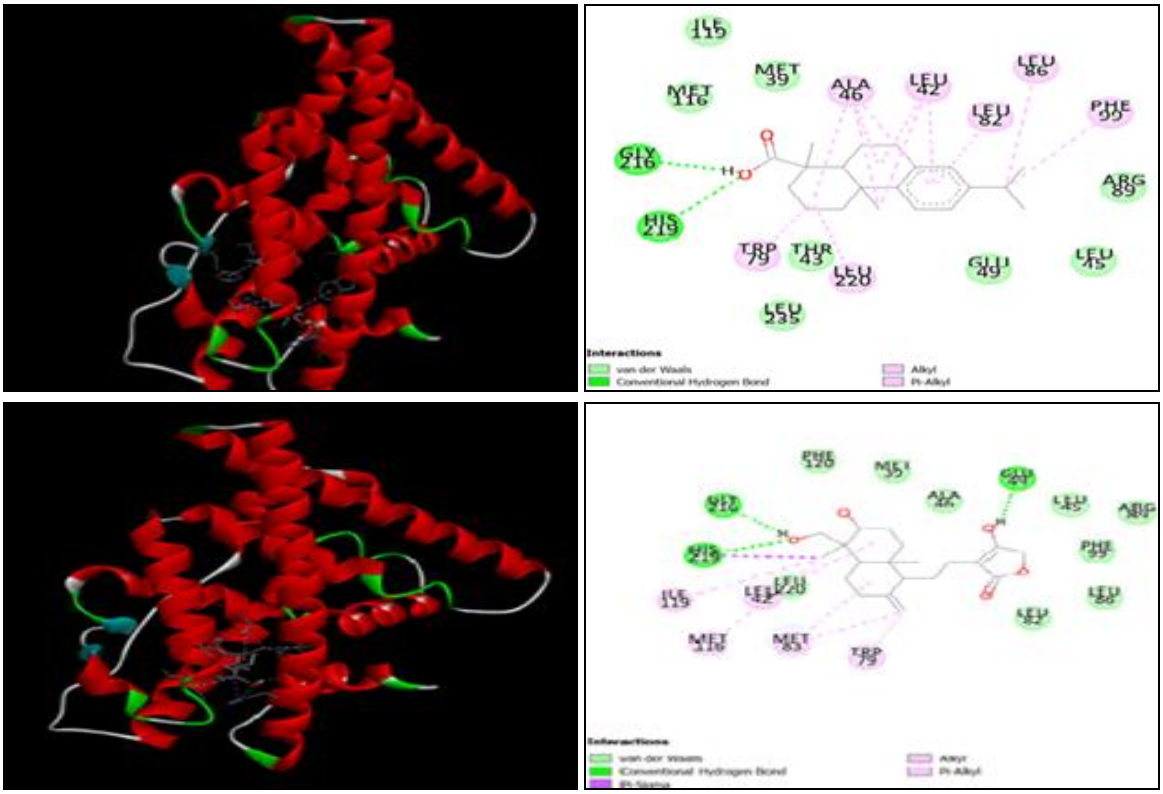

FIG. 3: DOCKING ANALYSIS OF ANDROGRAPHOLIDE WITH ESTROGEN RECEPTORS

Toxicity Profile of Selected Compounds: Table 3 shows that toxicity profile of the compounds palustric acid and andrographolide non-toxic in AMES test and LD50 in rats.

TABLE 3: TOXICITY PROFILE OF SELECTED COMPOUNDS

Name of the ligand	Oral rat LD50 data set	Ames mutagen city data set
Palustric acid	1.87	Mutagen city Negative
Andrographolide	4	Mutagen city Negative

Molecular Dynamics Simulation Studies: At the end of the 100 ns simulation, the ER-Palustric acid complex was observed to be stabilized at around 0.16 nm. This was lower compared to the RMSD deviation of around 0.21 nm for the ER-Andrographolide complex. **Fig. 5** depicts the

comparative RMSD plot for the two complexes. The stability of interactions was found to be more stable for the ER-Palustric acid complex. The RMSD for the ligand Palustric acid was relatively lower (0.15 nm) compared to Andrographolide. The RMSF fluctuation for both complexes was less than 0.2 nm depicting the stability of the complexes **Fig. 6.**

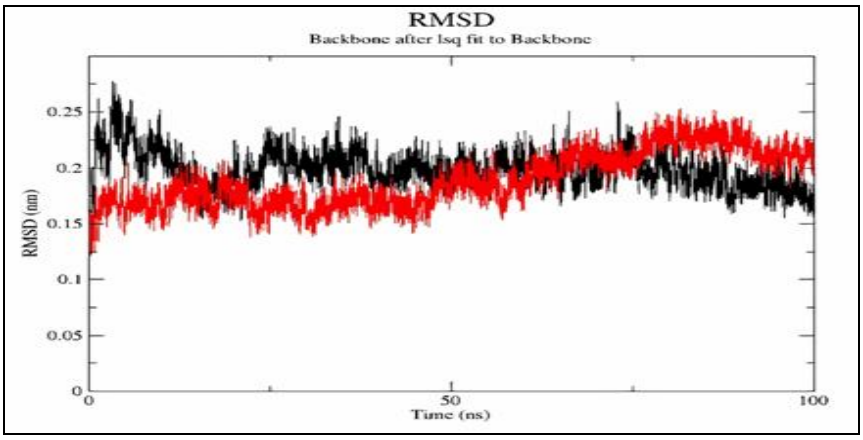

FIG. 4: COMBINED RMSD PLOT FOR ER-PALUSTRIC ACID AND ER-ANDROGRAPHOLIDE COMPLEXES

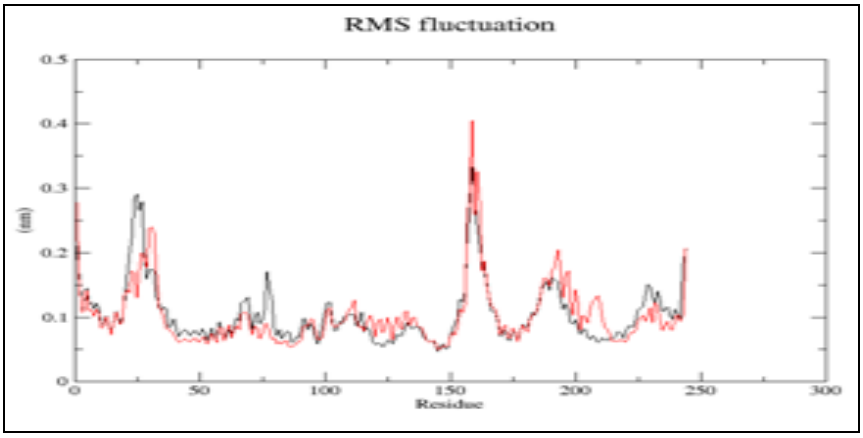

FIG. 5: COMBINED RMSF PLOT FOR ER-PALUSTRIC ACID AND ER-ANDROGRAPHOLIDE COMPLEXES

A stable value for R_g was observed for both complexes. Both the protein complexes were seen to remain compact over the 100 ns time scale. A stable value of approximately 1.9 nm was seen for both complexes.

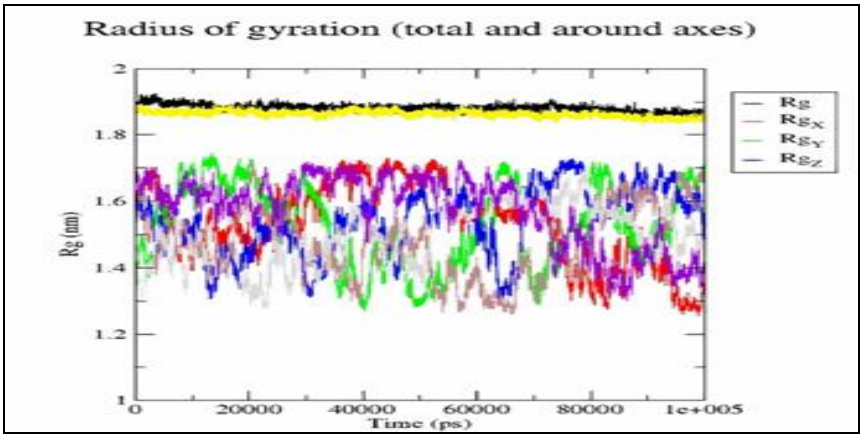

FIG. 6: COMBINED RG PLOT FOR ER-PALUSTRIC ACID AND ER-ANDROGRAPHOLIDE COMPLEXES

Interaction Analysis: The non-bonded interaction energies were evaluated for the two complexes. For both the complexes, no much differences were computed with respect to short-range lennard-Jones energy and potential energy. Although, the ER-Palustric acid complex shower a higher total

interaction energy between the protein and the ligand than the ER-Andrographolide complex. This suggests that Palustric acid has a better stable binding than the other ligands, which is also confirmed by the above results. Other parameters have also been listed in **Table 4.**

TABLE 4: PROTEIN-LIGAND INTERACTION ENERGIES FOR THE TWO COMPLEXES

Parameters	MD_1	MD_2
Short range coulombic interaction energy	-57.4723 kj mol - ¹	-13.6147 kj mol - ¹
Short range lennard – Jones energy	-168.543 kj mol - ¹	-159.742 kj mol - ¹
Total Interaction energy	-226.0153 kj mol - ¹	-173.3567 kj mol - ¹
Potential energy	-573132 kj mol - ¹	-572553 kj mol - ¹
Kinetic energy	11.4322 kj mol - ¹	5.70952 kj mol - ¹

DISCUSSION: Breast cancer is known as capital punishment and is the second most significant reason for death in the world. The proportion of Breast cancer malignant growth in is one of every nine if there should arise an occurrence of ladies [20]. Main source of Breast cancer disease is over articulation of estrogen hormone [21]. Therefore ER is utilized as an objective for anticipation of Breast cancer malignant growth. Tamoxifen is the main bad guy of ER and is monetarily accessible as a medication to control Breast cancer malignant growth [22]. It ties in with Arg394 and blocks the capacity of estrogen receptors and restrains the capacity of ER [23]. Docking permits the researcher to practically screen a data set of mixtures and foresees the most grounded covers in light of different scoring capacities.

It investigates manners by which two atoms, for example, drugs and a protein Human estrogen receptor, fit together and dock to each other well, similar to bits of a three-layered jigsaw puzzle. The particles restricting a receptor restrain its capacity and accordingly go about as medication. In ongoing exploration, PC helped drug planning (CADD) assists the scientist with diminishing the time and cash for drug planning projects [24]. Molecular docking is extremely useful in concentrating on the collaborations of ligand atoms with the objective protein before its *in-vitro* combination. Docking is performed through PC programs like Maestro [25]. To screen out the viable bioactive mixtures from *Ocimum basilicum* to be specific palustric acid and andrographolide, which might be possible inhibitors of estrogen receptor (ER) for looking through a medication against breast disease. A wide scope of docking scores was found during molecular docking. palustric acid and andrographolide showed the docking score - 8.95,-8.91separately. Among these mixtures, palustric acid shows the most noteworthydocking score and dynamics studies.

CONCLUSION: The GC-MS analysis of the *Ocimum basilicum* Aqueous Leaf Extract revealed the presence of 45 compounds among the two compounds chosen by the rule of five. The docking analysis has exhibited, and binding affinities of 2 Palustric acids, and Andrographolide are -8.95 and-8.44 Kcal/mol, respectively. The molecular dynamics and toxicity properties showed Palustric acid and andrographolide satisfied all rules. The results revealed that the compounds present in *Ocimum basilicum* Aqueous Leaf Extract could inhibit the Estrogen receptor.

ACKNOWLEDGMENT: The authors thank St Joseph's College for providing the software and the support for carrying out the work.

CONFLICTS OF INTERESTS: The authors declare that they have no competing interests.

REFERENCE:

1. Ee C, Cave AE, Naidoo D, Bilinski K & Boyages J: Weight management barriers and facilitators after breast cancer in Australian women: a national survey. BMC Women's Health 2020; 20(1): 1-10.
2. Rodríguez-Palacios DÁ, Colorado-Yohar SM, Velten M, Vaamonde-Martín RJ, Ballesta M & Chirlaque MD: Incidence and Trend of Type I and II Endometrial Cancer in Women from Two Population-Based European Cancer Registries (1998–2012). Intern Journal of Environmental Research and Public Health 2022; 19(7): 3789.
3. Rahib L, Wehner MR, Matrisian LM & Nead KT: Estimated projection of US cancer incidence and death to 2040. JAMA Network Open 2021; 4(4): e214708-e214708.
4. White MC, Kavanaugh-Lynch MMH, Davis-Patterson S & Buermeyer N: An expanded agenda for the primary prevention of breast cancer: Charting a course for the future. International Journal of Environmental Research and Public Health 2020; 17(3): 714.
5. Liu XY, Li P, Li XS, Simoncini T & Cheng Y: 17β-Estradiolnongenomically induces vasodilation is enhanced

by promoting phosphorylation of endophilin A2. Gynecological Endocrinology 2022; 38(8): 644-650.
6. Soumyakrishnan S & Sreepriya M: The Good, Better And Best About Selective Estrogen Receptor Modulators As Novel Guardians Against Osteoporosis. Plant Cell Biotechnology and Molecular Biology 2022; 15-30.
7. Patel JM & Jeselsohn RM: Estrogen Receptor Alpha and Mutations in Breast Cancer. In Nuclear Receptors in Human Health and Disease 2022; 171-19.
8. Thang NX, Yoo S, La H, Lee H, Park C, Park KS & Hong K: Epigenetic Factors as Etiological Agents, Diagnostic Markers, and Therapeutic Targets for Luminal Breast Cancer. Biomedicines 2022; 10(4): 748.
9. Lu Y, Tong Y, Chen X & Shen K: Association of biomarker discrepancy and treatment decision, disease outcome in recurrent/metastatic breast cancer patients. Frontiers in Oncology 2021; 11: 2573.
10. Barik A, Ray SK, Byram PK, Sinha R & Chakravorty N: Extensive early mineralization of pre-osteoblasts, inhibition of osteoclastogenesis and faster peri-implant bone healing in osteoporotic rat model: principle effectiveness of bone-specific delivery of Tibolone as evaluated *in-vitro* and *in-vivo*. Biomedical Materials 2020; 5(6): 064102.
11. Jung SY, Jeong J, Shin SH and Kwon Y: The invasive lobular carcinoma as a prototype luminal A breast cancer: A retrospective cohort study, BMC Cancer, 10, 2018, 664
12. Guedes IA, Barreto A. Marinho D, Krempser E, Kuenemann MA, Sperandio O and Miteva MA: New machine learning and physics-based scoring functions for drug discovery. Scientific reports 2021; 11(1): 1-19.
13. Surabhi S & Singh BK: Computer aided drug design: an overview. Journal of Drug delivery and Therapeutics, 2018; 8(5): 504-509.
14. Al-Husseini ZNO & Neema BZ: Pharmaceutical Application Of Molecular Docking In Drugs, Optimization, Characterization And Synthesis 2022.
15. Torres, P. H., Sodero, A. C., Jofily, P., & Silva-Jr, F. P. (2019). Key topics in molecular docking for drug design. International journal of molecular sciences, 20(18), 4574.
16. Rangel, E. M., e Silva, E. F., Macagnan, K. L., Ribeiro, L. V., Cardoso, T. F., &Garcez, D. K. (2022). The use of bacteria for bioremediation of environments contaminated with toluene: a molecular docking analysis. Ciência e Natura, 44, e17-e17.
17. Vsdna NS, Muniappan M, Kannan I and Viswanathan S (2017). Phytochemical analysis and docking study of compounds present in a polyherbal preparation used in the treatment of dermatophytosis. Current Medi Mycol 3(4): 6.
18. Kecel-Gunduz, S., Bicak, B., Kokcu, Y., Ozel, A., &Akyuz, S. (2020). The Interaction of Ile-Phe Dipeptide with Phosphatidylinositide 3-Kinase (PI3K): Molecular Dynamics and Molecular Docking Studies. Natural and Engineering Sciences.
19. Lee, M., Kwon, S., & Lee, W. B. (2022). Structure and Property of Alkylated Graphene Oxide Depending on the Chain Length: Grand Canonical Monte Carlo-Molecular Dynamics Approach. The Journal of Physical Chemistry C, 126(29), 12178-12183.
20. Ullah, Z., Khan, M. N., Din, Z. U., &Afaq, S. (2021). Breast Cancer Awareness and Associated Factors Amongst Women in Peshawar, Pakistan: A Cross-Sectional Study. Breast Cancer: Basic and Clinical Research, 15, 11782234211025346.
21. Daraei A, Izadi P, Khorasani G, Nafissi N, Naghizadeh, MM, Meysamie A & Tavakkoly-Bazzaz J: A methylation signature at the CpG island promoter of estrogen receptor beta (ER-β) in breasts of women may be an early footmark of lack of breastfeeding and nulliparity. Pathology-Research and Practice 2021; 218: 153328.
22. Raman V: Inhibition of metabolism and induction of apoptosis in triple negative breast cancer cells by lippiaoriganoides plant extracts (Doctoral dissertation, Purdue University Graduate School). (2019).
23. Gonzalez T: Role of Environmental Estrogens and Acquired Endocrine Resistance in Breast Cancer and Implications for Treatment with Novel Antiestrogens (Doctoral dissertation) 2018.
24. Jain S, Amin SA, Adhikari N, Jha T & Gayen S: Good and bad molecular fingerprints for human rhinovirus 3C protease inhibition: Identification, validation, and application in designing of new inhibitors through Monte Carlo-based QSAR study. Journal of Biomolecular Structure and Dynamics 2020; 38(1): 66-77.

How to cite this article:
Monica AA: Identification and validation of palustric acid and andrographolide from *Ocimum basilicum* leaf as a promising breast cancer inhibitor: an *in-vitro* and *in-silico* analysis. Int J Pharm Sci & Res 2023; 14(6): 2899-06. doi: 10.13040/IJPSR.0975-8232.14(6). 2899-06.