Gopinathan Narasimhan. et al. /Asian Journal of Research in Chemistry and Pharmaceutical Sciences. 7(2), 2019, 398-401.

Research Article

ISSN: 2349 - 7106



Asian Journal of Research in Chemistry and Pharmaceutical Sciences

Journal home page: www.ajrcps.com



SCREENING OF FEW PHYTOCHEMICALS OF COUROUPITA GUIANENSIS LINN AGAINST BREAST CANCER BY AN INSILICO APPROACH - A FIRSTHAND TREND

Gopinathan Narasimhan*¹, Yerramilli Lalitha Sravya¹, Chitra Krishnan¹, D. Chamundeeswari¹ ¹*Faculty of Pharmacy, Sri Ramachandra Institute of Higher Education and Research, Porur, Chennai, Tamilnadu 600116, India.

ABSTRACT

Cancer is distributed over a large area whereas it is threat to humanity. In prevention and treatment of cancer, plants play an important role. The scientific name of Nagalingam is *Couroupita guianensis* Linn (Family: Lecythidaceae) a tree found throughout the plains of India. It inhibits the growth of microorganisms and show larvicidal activity against vectors. Among female fatal breed of cancers is breast Cancer. It is the cancer originating from intramural lining of milk ducts a tissue of breast, particularly which impart the ducts with milk. Hsp90 is an abundant protein in mammalian cells. Hsp90 plays a major role in breast neoplasia, which is aboundant in breat tissue. **Methodology:** The method involved the ligand preparation, protein preparation, grid generation and docking against the target using GLIDE - Maestro 2018. The sixteen active constituents present were the ligands. The target protein is 3TUH downloaded from protein data bank. **Results and discussion:** The docking score were Isatin -5.48, Indigo -5.29, Coup2 -5.23, Indirubin-5.25, Calotronaphthalene -5.06, Coup -4.99, Alpha Amyrin -4.94, Nerol-4.75, Betasitosterol - 4.74, Campesterol-4.68, Eugenol -4.61, Tryptanthrin -4.31, Benzyl Alcohol -4.10, Betaamyrin -3.07 and Farnesol - 3.06. The protein is validated before docking with ligand 3TUH_TUH_A_1 with score of -9.53 and standard dauxorubicin with docking value of - 6.51. **Conclusion:** Among the docked compound, isatin had good docking score comparable to standard. It had shown interaction with the ASN 51 like standard and interacted with LYS 58 like the validated compound. In future scope of work the isatin can be screened against breast cancer.

KEYWORDS

Couroupita guianensis Linn, GLIDE, Heat shock protein and Active principles docking.

Author for Correspondence:

Gopinathan Narasimhan, Faculty of Pharmacy, Sri Ramachandra Institute of Higher Education and Research, Porur, Chennai, Tamilnadu - 600116, India.

Email: gopinathan.n@sriramachandra.edu.in

Available online: www.uptodateresearchpublication.com

INTRODUCTON

Nagalingam, is a tree found throughout the plains of India is scientifically called as *Couroupita guianensis* Linn (Family: Lecythidaceae) is used to cure cold, intestinal gas formation, stomachache and have immunomodulatory activity. It inhibits the growth of microorganisms and show larvicidal activity against vectors. It is habitually known as cannonball tree, Sal tree or Ayahuma tree and vernacular name varies according to the different April – June 398

places. Traditionally, it shares its importance in treatment of animals. It is augmented with a quantity of active component like isatin, linalool, eugenol, farnesol, beta sitosterol, nerol, linoleic acid, benzyl alcohol, 7 methoxy 4-methyl coumarin, trypthantrin, quercitin, terpineol, indirubin, benzthiazole, indigo, hexadecanoic acid, limonene, alpha amyrin, beta amyrin, beta amyrin palmitate, stigmasterol, campesterol, beta carotene. The extracts of Couroupita guianensis shows a variety of pharmacological activities which accomplish further exploration to isolate active compounds with therapeutic value, further they can be castoff for the creation of new drug moieties for the treatment of numerous ailments. The tree is of botanical curiosity and it possess various activities like anxiolytic, anti-microbial, wound healing, antiulcer, anti-oxidant, anti-diabetic, anti-radical, immunomodulatory anti-bacterial. activity. anti-fungal, expectorant activity, anti-biofilm properties, analgesic, anti-inflammatory, antidepressant, antiseptic, antipyretic, anti-fertility, anti diarrhoeal, anti-protozoal and anti-cancer activity.

A new active chemo preventive molecule provide by plant which play a vital role in a wide spread threat to humanity. Among female fatal breed of cancers is breast Cancer. It is the cancer originating intramural lining of milk ducts a tissue of from breast, particularly which impart the ducts with milk. In women, the breast cancer is 22.9% among the other cancers. In women 13.7 % death due to cancer, worldwide four and half lakhs death caused by breast cancer. Mammalian cells are abundant with HSP 90. Hsp90 plays a major role in breast neoplasia, which is abundant in breast tissue. Proteins from degradation, oxidative stress, hypoxia, and thermal stress are protected by it. In cancer members of the hsp70, hsp27 and hsp90 families proposed to play a defined role. They are significant regulators of cellular proliferation, differentiation during the development of cancer.

HER2 tyrosine kinase, antiapoptotic kinase, Raf-1 MAP kinase, angiogenesis transcription factor, tumor suppressor p53 protein, estrogen receptors etc. are the variety of proteins that interact with

Available online: www.uptodateresearchpublication.com

HSP 90 that plays a key role in breast neoplasia. The aim and objective of the present study is to dock the few active principles of *Couroupita guianensis* Linn against the breast cancer in the in silico approach.

MATERIAL AND METHODS Methodology

Ligand preparation

3D chemical structure of selected bioactive compounds such as isatin, eugenol, farnesol, beta sitosterol, nerol, benzyl alcohol, trypthantrin, indirubin, indigo, alpha amyrin, beta amyrin, stigmasterol, campesterol were downloaded from PubChem database in sdf format • Retrieved into glide software • Ligand was prepared using Ligprep wizard of glide software.

Protein preparation

3D crystalline structure of protein [PDB ID is 3TUH] was acquired from protein data bank. It was prepared using prep wizard of glide software. Grid was generated using the glide grid generation wizard. It is the crystal structure of HSP90 protein a N terminal domain, which is complexed with inhibitor ganetespib. The organism is homosapien. Its X- ray diffraction has resolution of 1.8A. It is heat shock protein HSP-90 alpha with A and B chains. The B chain is removed during the protein preparation.

Ligand docking

It was performed using ligand docking - Glide. Analysis of docked complex.

RESULTS AND DISCUSSION

The validation is performed using the ligand which is binded in the target already. It has given good docking score of -9.43. Pie cation interaction is between the phenyl ring and LYS 58 residues. The hydrogen bonds formed are two. The polar OH of ligand formed hydrogen bond with ASP 93 and another hydrogen bond is formed with GLY 97 of protein and NH of triazole ring of the compound. Third hydrogen bond is formed with water molecule in the protein.

The OH of benzyl alcohol formed one hydrogen bond with the target at ASN 51 residue. The bond Gopinathan Narasimhan. et al. /Asian Journal of Research in Chemistry and Pharmaceutical Sciences. 7(2), 2019, 398-401.

length is 1.99°A. The OH at 3rd position of betasitosterol formed hydrogen bond with LYS 58. The OH of camper sterol formed an hydrogen bond with PHE 138. The Coup had Pi interaction with LYS 58. Eugenol polar OH group formed hydrogen bond with ASP 93. The OH of farnesol formed hydrogen bond with LYS 58. The isatin formed two hydrogen bonds with the target protein. The NH of isatin formed hydrogen bond with ASN 51. The carbonyl of isatin next to nitrogen atom formed hydrogen bond with LYS 58. Nerol formed two hydrogen bond with the protein. The OH of nerol formed a hydrogen bond with ASP 93 and GLY 97. Trytanthrin formed Pie interaction with LYS 58. alpha amyrin had no interaction.

The standard dauxirubocin is docked and had binding energy of -6.51 with five hydrogen bonds. The C ring of doxorubicin carbonyl oxygen form hydrogen bond with LYs 112. The NH2 of doxorubicin formed a hydrogen bond with Lys 112. OH of doxorubicin [CO-CH2_OH] formed hydrogen bond with ASN 106. The OH of doxorubicin formed two hydrogen bond with ASN 51 and PHE 138.

Constituents against 51 011		
S.No	Active constituent	Docking score
1	Doxirubocin	-6.51
2	3TUH_TUH_A_1	-9.43
3	Isatin	-5.48
4	Indigo	-5.29
5	Coup2	-5.23
6	Indirubin	-5.25
7	Calotronaphthalene	-5.06
8	Coup	-4.99
9	Alpha Amyrin	-4.94
10	Nerol	-4.75
11	Betasitosterol	-4.74
12	Campesterol	-4.68
13	Eugenol	-4.61
14	Tryptanthrin	-4.31
15	Benzyl Alcohol	-4.10
16	Betaamyrin	-3.07
17	Farnesol	-3.06

Table No.1: Docking result of Active Constituents against 3TUH



Figure No.1: Validation of the protein 3TUH Figure No.2: Docking posture of standard Doxirubocin with protein -3TUH

Available online: www.uptodateresearchpublication.com

April – June

Gopinathan Narasimhan. et al. /Asian Journal of Research in Chemistry and Pharmaceutical Sciences. 7(2), 2019, 398-401.



Figure No.3: Docking poses of isatin with protein 3TUH

CONCLUSION

Among the docked compound, isatin had good docking score comparable to standard. It had shown interaction with the ASN 51 like standard and interacted with LYS 58 like the validated compound. The benzyl alcohol showed the same interaction at ASN 51 residue of protein like standard. The nerol and Eugenol showed the interaction like the validated compound. In future scope of work the isatin can be screened against breast cancer.

ACKNOWLEDGEMENT

We thank the management of Sri Ramachandra Institute of Higher Education and Research deemed to be university for providing the needed facility to carry out this research work.

CONFLICT OF INTEREST

We declare that we have no conflict of interest.

BIBILIOGRAPHY

- 1. Conroy S E and Latchman D S. Do heat shock proteins have a role in breast cancer? Medical Molecular Biology Unit, Department of Molecular Pathology, *British Journal of Cancer*, 74(5), 1996, 717-721.
- 2. Stuart K. Calderwood. Heat shock proteins in breast cancer progression - A suitable case for treatment? Molecular and Cellular Radiation Oncology, Beth Israel Deaconess Medical Center, Harvard Medical School, *Int. J. Hyperthermia*, 26(7), 2010, 681-685.
- 3. Suman Chatterjee, Timothy F. Burns. Targeting Heat Shock Proteins in Cancer: A Promising Therapeutic Approach, *International Journal of Molecular Sciences*, 18(19), 2017, E1978.
- 4. Lee Su Kim, Jun Ho Kim. Heat Shock Protein as Molecular Targets for Breast Cancer Therapeutics, *Journal of Breast Cancer*, 14(3), 2011, 167-174.
- 5. Santosh Kumar, Sharma Vivek P. Chavda: "Cannon Ball Tree"- The Alchemist Plant, *Innoriginal International Journal of Sciences*, 2(5), 2015, 6-9.
- 6. Raja Sundararajan and Ravindranadh Koduru. A complete profile on Couroupita guianensis - Traditional uses, Pharamacological activities and phytoconstituents, *Pharmacophore (An International Research Journal)*, 5(1), 2014, 147-159.

Please cite this article in press as: Gopinathan Narasimhan *et al.* Screening of few phytochemicals of *Couroupita guianensis* Linn against breast cancer by an Insilico approach - a firsthand trend, *Asian Journal of Research in Chemistry and Pharmaceutical Sciences*, 7(2), 2019, 398-401.