ISSN PRINT 2319 1775 Online 2320 7876

Research paper UGC CARE Listed (Group -I) Journal Volume 11, S Iss 3, Dec 2022

Computational Approach In Search Of Therapeutic For Colorectal Cancer

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ABSTRACT

Colorectal cancer (CRC) is the second most lethal cancer in the world. Due to late discovery, a high recurrence rate, and multi-drug resistance, CRC care is difficult. Herbs and spices used in cooking have been demonstrated to include CRC protective effectors and can even be utilised as an anti-CRC adjuvant treatment when taken in large dosages. Herbs and spices include several bioactive chemicals that have numerous health benefits. These herbs and spices' chemopreventive activities are primarily mediated by multiple routes, including caspase activation, the extrinsic apoptotic pathway, and the modulation of ER-stress-induced apoptosis. As a result, Ginger (Zingiber officinale) was chosen for this study and studied for

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its chemoprotective or chemotherapeutic effects in CRC treatment, as well as the underlying molecular mechanisms of action. This study first reviewed the molecular base of CRC formation, followed by culinary and traditional usage, current scientific research, and publications of chosen spices and plants.

Key words: Colorectal cancer, Zingiber officinale, Protein prediction, Molecular Docking.

1. Introduction

Cancer is a primary cause of mortality that has a considerable impact on every country's life expectancy. Colorectal cancer (CRC) is the third most often diagnosed and second most lethal disease worldwide, accounting for roughly 9.39% of all cancer deaths in 2020. The global incidence of CRC is anticipated to increase by 2035 due to the rapid increase in diagnosed cases among the elderly. The number of CRC patients detected in developing nations is likely to grow. The word CRC refers to cancer that develops in the large intestine and rectum as a result of improper proliferation of glandular epithelial cells. This happens when epithelial cells undergo a series of genetic or epigenetic changes that provide them a selective advantage in hyper-proliferation [1]. CRC is divided into four stages, much like any other tumour or cancer: stage 0 (carcinoma in situ) through stage IV. Surgery is the standard treatment method for stages 0 to II CRC, whereas surgery plus adjuvant chemotherapy are required for stage III, and recurrence is required for stage IV. CRC is treated with surgery, chemotherapy, and targeted treatment [2].

Only 40% of CRC is discovered in its early stages, and CRC can relapse following therapy. The Food and Drug Administration (FDA) has licenced at least 30 different medications for CRC therapy, which are used either alone or in combination with other treatments [3]. These chemotherapeutic medicines are administered to cancer cells while also harming healthy cells. As a result, these medicines cause tiredness, headache, muscular discomfort, stomach pain, diarrhoea and vomiting, sore throat, blood irregularities, constipation, neurological damage, skin changes, memory issues, lack of appetite, and hair loss [4].

Despite the fact that overall survival of individuals with advanced CRC has increased in recent decades as a result of new chemotherapy regimens, current systemic chemotherapies developed resistance in nearly all patients with CRC, limiting the therapeutic efficacy of anti-cancer medicines and ultimately leading to chemotherapy failure. In today's clinical practise,

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chemotherapeutic drug resistance is a key concern in CRC treatment. Aside from this constraint, access to CRC diagnosis and treatment for survival is less accessible in underdeveloped nations, particularly in rural areas, where about 44% of the world's population now lives. As a result, over half of the world's population lacks access to diagnosis and treatment [5].

Ginger (Zingiber officinale Rosc.) is a tropical and subtropical plant that originated in South-East Asia and has since spread to many areas of the world. It has been grown for thousands of years as a spice and for medicinal uses. The ginger plant has a perennial, tuberous base or rhizome; the stems are 2 or 3 feet tall, upright, oblique, spherical, and enveloped by the smooth sheaths of the leaves [6]. Ginger rhizome is commonly consumed as a fresh paste, dried powder, syrup-preserved slices, candy (crystallised ginger), or as a tea flavour. Fresh ginger is used in many nations, particularly India and China, to produce vegetable and meat dishes, as well as to flavour drinks and a variety of other food preparations. Since ancient times, the subterranean stem or rhizome of this plant has been utilised as a remedy in Asian, Indian, and Arabic herbal traditions [7]. For more than 2500 years, it has been used widely in China for headaches, nausea, and colds, as well as in the Mediterranean and Western areas of herbal medical practise for the treatment of arthritis, rheumatological diseases, and muscle pain. Its use in inflammatory disorders is compatible with the anti-inflammatory properties of its constituents in vitro. It has also been proposed as a therapy for a variety of other ailments such as atherosclerosis, migraine headaches, rheumatoid arthritis, excessive cholesterol, ulcers, depression, and impotence [8]. In addition to its therapeutic properties, ginger is widely used as a cooking spice and is said to assist with the common cold, flu-like symptoms, and even painful menstrual periods. Because of these qualities, it has received a lot of interest as a botanical dietary supplement in the United States and Europe in recent years, particularly for its use in the treatment of chronic inflammatory disorders. Several population-based studies demonstrate that individuals in South East Asian nations had a considerably lower incidence of colon, gastrointestinal, prostate, breast, and other cancers than their Western counterparts, and it is believed that dietary ingredients play a key role in prevention [9].

Ginger (Zingiber officinale Roscoe) was chosen for this study and studied for its chemoprotective or chemotherapeutic effects in CRC care, as well as the underlying molecular mechanisms of action. This study began with a thorough discussion of the

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molecular foundation of CRC formation, followed by culinary and traditional usage, current scientific research, and articles on the effects of various herbs and spices on malignancies.

2. Materials and Methods

2.1 Protein Preparation

The RCSB Protein Data Bank was used to get the three-dimensional crystal structures of the target proteins, 7NC0, engaged in several cancer pathways. The data bank's 7NC0 structure has a resolution of 2.20. Prior to molecular docking, all water molecules and pre-existing small molecules attached to the proteins were eliminated. The target proteins' structures were cleaned and energy was decreased before computing Gasteiger charges and adding polar hydrogens with the PyRx 0.8 virtual screening programme [10].

2.2 Ligand Preparation

Based on the literature, we selected some of the phytochemical structures of known antioxidant action. The selective ligands were retrieved in Three-dimensional form from IMPPAT, the largest digital database on phytochemicals of Indian medicinal plants. The selective ligands were listed in Table 1 [11].

2.3 Protein Binding site Prediction

The potential binding pockets of the proteins were collected from the Galaxy WEB server, which gives surface pockets and inner cavities of the provided protein pdb file [12]. This server also measures the binding pockets' area and volume. The docking programme selects and specifies the residues highlighted in the sequence of the chosen pocket [13].

2.4 Molecular Docking

Molecular docking was used to evaluate which plant compounds interacted best with the identified cancer targets based on binding free energies and affinity, as well as those exhibiting significant hydrophobic interactions and hydrogen bonds. The molecular docking investigation of phytocompounds targeting cancer proteins was performed using the PyRx 0.8 programme. A grid box was created around the protein's designated binding residues, to which the ligands were docked. Nine poses of each ligand docked to the active site of the

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cancer target protein were produced and sorted in descending order based on the negative binding energy value. The visualisation programme, PyMOL 2.4 from Schrodinger, and the BIOVIA discovery studio visualise tools were used to further examine these compounds.

3 Results

3.1 Protein Preparation

The humanised A33 Fab variant, an immunotherapy candidate for colorectal cancer with PDB ID 7NC0 is visualized using UCSF Chimera a visualization software and is represented in the Figure 1.

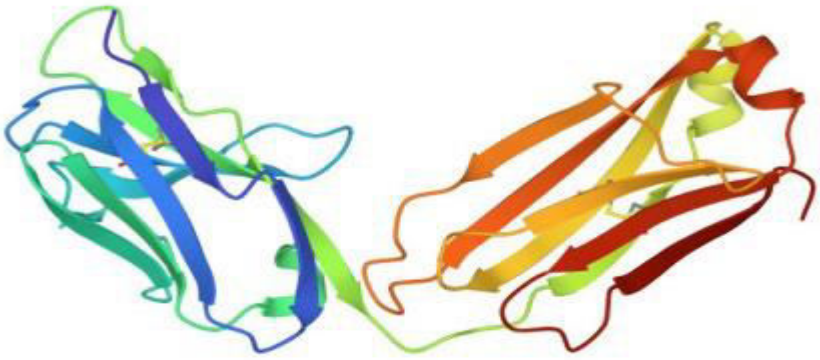
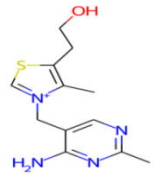
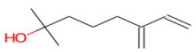


Figure 1: The 3D structure of the humanised A33 Fab C226S variant

3.2 Ligand Preparation

Using the IMPPAT database the Phytochemical compound of Zingiber officinale plant were downloaded in pdb format.

Table 1. Phytochemical Name and Structure obtained from IMPPAT Database

IMPPAT Phytochemical Identifier	Phytochemical Name	Structure
IMPHY000005	Thiamine	
IMPHY000022	Myrcenol	

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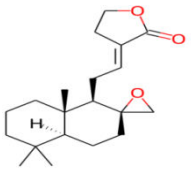
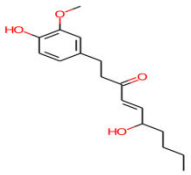
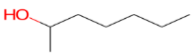
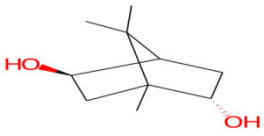
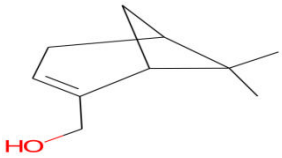
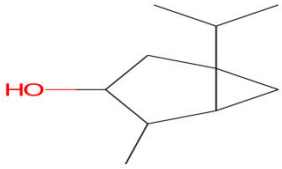
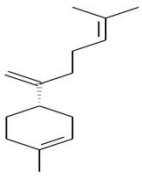
IMPHY000028	Galanolactone	
IMPHY000047	6-Hydroxyshogaol	
IMPHY000084	2-Heptanol	
IMPHY000438	Angelicoidenol	
IMPHY000099	Myrtenol	
IMPHY000173	Thujyl alcohol	
IMPHY000399	beta-Bisabolene	

3.3 Binding site Prediction

Galaxy WEB was used to obtain the binding pocket residues of the protein that are responsible for the protein-ligand interaction. The residues recovered were 91H, 92W, 93S, 94Y, and 96L.

3.4 Molecular docking interactions between 7NC0 and selective ligands.

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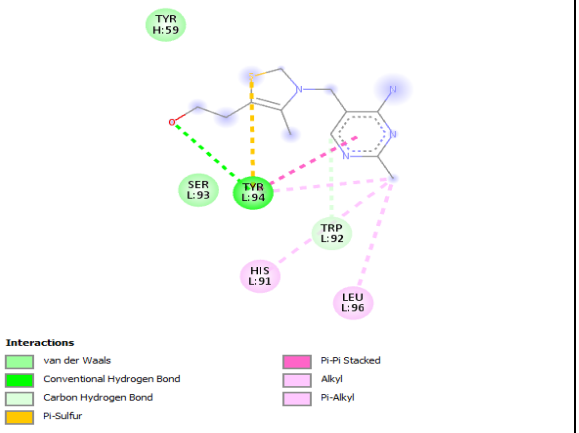
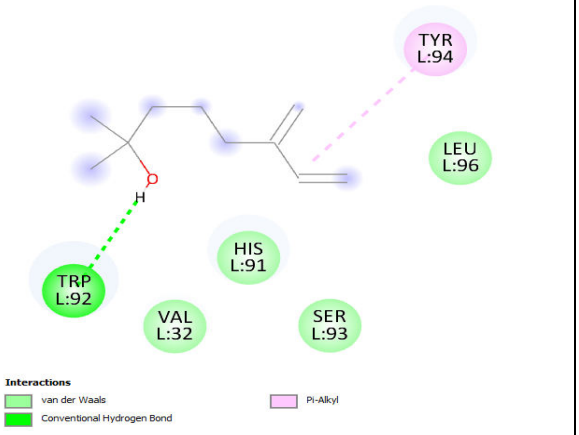
Molecular docking is a popular drug discovery approach with few to no negative side effects. It is a two-step process that begins with geometrical optimization of the ligand and target biomolecule. The conformations in the receptor-identified active area are then rated based on their score, which varies depending on the procedures used to generate them from programme to programme. As a result, selected ligands interacts with 7NC0 via hydrogen bond 91H, 92W, 93S, 94Y and 96L with other amino acid residues. These findings suggest that Myrtenol binding to 7NC0 is quite strong in comparison to others.

Table 2. Analyzing Molecular Docking Interaction

Protein ID	**Plant name**	**Ligand Name**	**Binding affinity**	**NO. of H-Bonds**	**2D Interaction**
7NC0	Zingiber officinale	Thiamine	-4.0	1	
		Myrcenol	-3.2	1	

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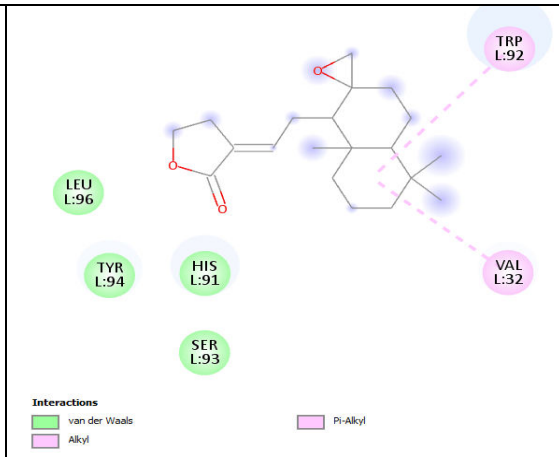
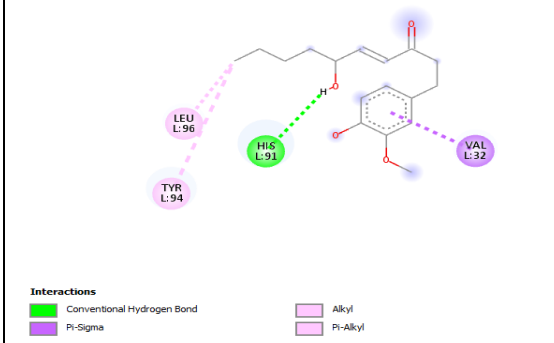
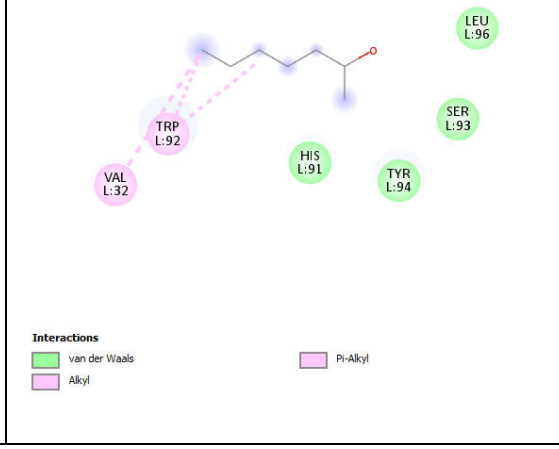
		Galanolactone	-4.8	0	
		6-Hydroxyshogaol	-4.4	1	
		2-Heptanol	-2.8	0	

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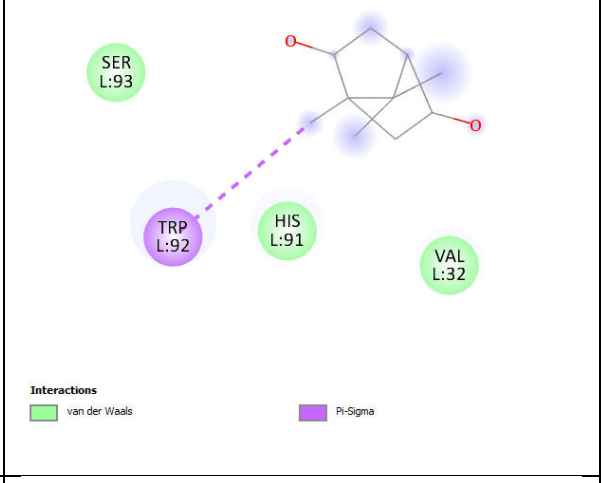
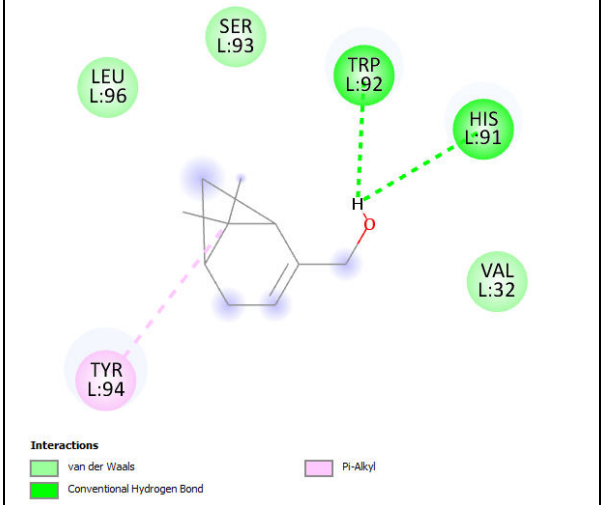
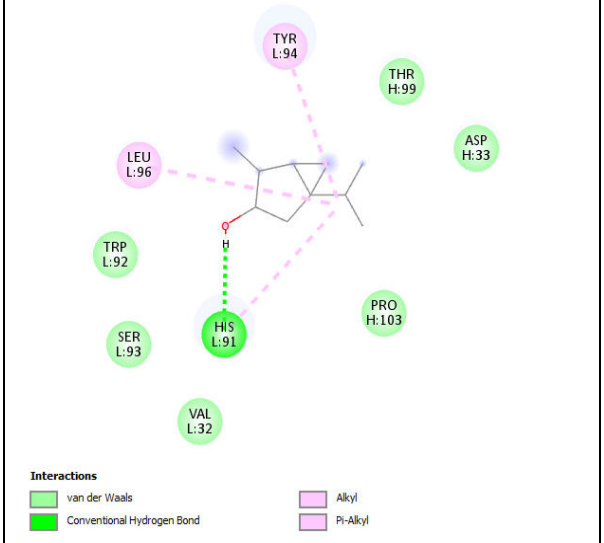
		Angelicoidenol	-3.2	0	
		Myrtenol	-3.4	2	
		Thujyl alcohol	-3.2	1	

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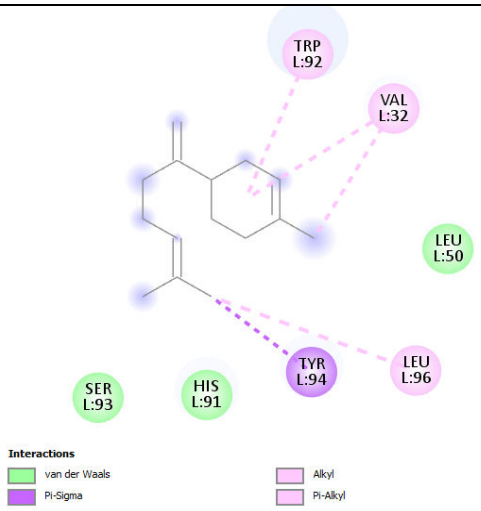
		beta-Bisabolene	-4.2	0	

4. Conclusion

The purpose of this study was to evaluate and examine the anti-cancer efficacy of Zingiber officinale in inhibiting the major proteins implicated in colorectal cancer development. Based on the Molecular Docking studies some Phytochemical compounds have good interaction with the targeted protein. In comparison to other ligands, the binding affinity of Myrtenol shows 2 Conventional Hydrogen Interaction with a Binding affinity of -3.4 kcal/mol.

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