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In Silico Evaluation of *Camptotheca acuminata* for Colorectal Cancer Treatment

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Abstract: Colorectal cancer (CRC) is still one of the main causes of cancer-related death globally, new therapeutic agents with increased effectiveness and fewer side effects must be investigated. The in-silico assessment of bioactive substances produced from *Camptothecaacuminata* in comparison with standard chemotherapeutic drugs for CRC treatment. Initially, bioactive compounds were identified from literature sources and screened based on drug-likeness and pharmacokinetic properties using ADME criteria. Potential protein targets associated with CRC were retrieved from relevant biological databases, and overlapping targets were identified to determine key therapeutic interactions. The binding affinity of particular drugs was evaluated using molecular docking research against critical CRC-associated proteins, followed by network pharmacology analysis to elucidate the underlying molecular mechanisms and pathways. The results demonstrated that several *Camptotheca acuminata* compounds exhibited significant binding affinity and comparable or superior interaction profiles relative to conventional chemotherapy drugs. Overall, this study highlights the promising role of natural compounds as alternative or complementary agents in CRC treatment and provides a computational foundation for further experimental validation and drug development.

Keywords: *Colorectal Cancer; Camptotheca Accuminata; Network Pharmacology; Toxicity Analysis; Phytocompounds.*

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I. INTRODUCTION

Colorectal cancer (CRC), also commonly referred to as bowel cancer, is also known as the fourth most incidental cancer, a malignant disease that arises from the epithelial lining of the colon or rectum. As one of the primary causes of cancer-related morbidity and mortality globally, it is one of the most important public health issues. According to data from the World Health Organization provided the data for colorectal cancer, affecting a million cases and new cases diagnosed annually by over 1.9 million and occurring in India consider approximately 64,000 to 65,000+ new cases reported in 2022 and death reports 38,367, the analysis Gender wise death report 40,430 cases in male vs. 24,433 cases in female and In India, the age-standardized incidence of colorectal cancer (CRC) rose from 4.3 per 100,000 males in 2008 to 7.2 in 2012. By 2026, it is predicted to increase by 37% for women and 60% for men.

CRC cancer combined with substantial medical, social, and economic impacts, highlights the critical need for early detection, prevention, and awareness. Polyps and tubular adenomas are examples of benign neoplasms that typically cause colorectal cancer (CRC). CRC develops gradually from abnormal growths on the inner lining of the colon or rectum that are commonly referred to as polyps. Polyps can develop into a tumour and spread into blood vessels, which makes it easier for cancer to spread.

The CRC has different stages involved they are four stages. The two major types of polyps—adenomatous polyps (adenomas) and serrated polyps—carry different levels of risk, this progression from benign to malignant growth is influenced by a complex interplay of genetic mutations, epigenetic changes, and environmental factors. Causes of colorectal cancer There are many risks associated with the occurrence of CRC. Specifically, CRC has been related to genetic mutations, such as the conversion of certain genes from proto-oncogenes to oncogenes A wide range of risk factors contributes to the development of colorectal cancer. Researchers are still investigating the reasons behind this shift, with suspected contributors including diet, lifestyle changes, micro biome alterations, and environmental exposures. Surgery, chemotherapy, radiation therapy, targeted therapy, and immune therapy are frequently combined in today's therapeutic techniques. Treatments are used to prevent the CRC or malignant to treat for the techniques involved and avoid the critical stages of cancer. Laparoscopic surgery, resection, palliative care, neoadjuvant chemotherapy, and radiotherapy are among the current option s for treating colorectal cancer.Ongoing research, improved access to healthcare, and comprehensive prevention strategies remain key to reducing incidence and enhancing survival

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outcomes. By increasing awareness and encouraging proactive health behaviour's, societies can make meaningful strides toward controlling and eventually reducing the impact of colorectal cancer.

II. MATERIAL AND METHODS

➢ *Identification of Comptotheca acuminata Compounds*

A total of 78 bioactive compounds from *Camptotheca acuminata* were retrieved from the literature (Li & Wang, 2014). The PubChem database (https://pubchem.ncbi.nlm.nih.gov/) provided the molecular structures of the substances. The absorption, distribution, metabolism, and excretion (ADME) characteristics and drug-likeness were assessed using the SwissADME (http://www.swissadme.ch/) program in order to screen possible therapeutic compounds.

According to Lipinski's Rule of Five, 32 compounds met the acceptance criteria, while 12 compounds were excluded due to predicted toxicity.

➢ *Compounds Target Prediction*

A drug's active ingredients use particular targets to carry out its biological effects. To determine these goals for CA's primary active ingredients, we employed canonical SMILES numbers to aid in target identification. SwissTargetPredictio(http://www.swisstargetprediction.ch/) was used to predict the potential targets for CA.

➢ *Collection of CRC Related Targets*

Colorectal cancer (CRC)–associated target genes were gathered from the Gene Cards database. (https://www.genecards.org/). A comprehensive search was performed using the primary keyword "colorectal cancer." To broaden the scope of target identification, additional CRC-related keywords obtained from previously published literature were also used to conduct separate searches within the same database. All retrieved gene entries were exported and combined into a unified dataset. Duplicate records were removed to eliminate redundancy.

➢ *Protein -Protein Interaction*

Camptotheca acuminata active component targets were crossed with CRC-related targets using VENNY 2.1 (https://bioinfogp.cnb.csic.es/tools/venny/) software to produce overlapping targets. The Search Tool for the Retrieval of Interacting Genes/Proteins (STRING) online database (https://string-db.org/) created the network protein–protein interaction network using the overlap targets between D. officinale active components targets and CRC-related targets, with the species restricted to "Homo sapiens," medium confidence of protein interaction data with a score > 0.400, and other default values. After downloading the interaction network data in TSV format, it was imported into Cytoscape 3.10.2 (https://cytoscape.org/) for topological analysis and visualisation. Hub proteins within the network were identified by calculating important topological metrics like degree centrality, betweenness centrality, and closeness centrality using Network Analyser.

Furthermore, the *Camptotheca acuminata* was applied to screen core target genes based on ranking algorithms.

➢ *GO and KEGG Enrichment Analysis*

The Shiny GO 0.77 database (https://bioinformatics.sdstate.edu/go/) Key compounds and disease targets were screened for GO and KEGG pathway enrichment analysis using a functional annotation and pathway enrichment tool; $p < 0.05$ was selected as the threshold to check for possible signalling pathways and anti-CRC mechanisms of action of CA drugs.

➢ *Molecular Docking by PyRx and Interaction Analysis*

The AutoDockWizard feature in PyRx (https://pyrx.sourceforge.io/) was used to do the molecular docking study. Important characteristics (Table 1) were collected and used to assess the binding affinity between the ligand and certain macromolecules. In this procedure, the ligand was loaded independently and the protein was loaded as a macromolecule. The loaded ligand was then optimised for maximum energy. Ensuring sufficient coverage of the entire surface area of the protein and the ligand was the aim. The parameters listed in the AutoDock Wizard feature of the PyRx program were used to start the docking operation. After the docking process, Discovery Studio (https://discover.3ds.com/discovery-studio-visualizer-download) visualisation was used to further investigate the ligand-protein docking complex for non-covalent interactions.

III. RESULT

➢ *Identification of Comptotheca acuminata Compounds*

The (table, 1) shows chemical information of the selected 32 active compounds was obtained from the PubChem database for each compound, the PubChem Compound ID (CID), compound name was retrieved.

➢ *Collection of CRC Related Targets*

To identify target genes associated with colorectal cancer, a comprehensive search was performed in the GeneCards database using the keyword "colorectal cancer." Additionally, 15 related keywords were extracted from a reference paper to expand the search, resulting in the retrieval of 284,834 genes.Common target genes were subsequently analysed using a Python script. Based on filtering criteria using average relevance score values, 50,959 genes were selected for further study. Gene abbreviations were specifically retrieved for *Homo sapiens* to ensure species-specific accuracy in the analysis.

➢ *Protein -Protein interaction*

The VENNY 2.1 software to cross 249 Comptotheca acuminata active component targets with 17767 CRC-related targets (Figure 1). This led to the attention of 242 common targets. A network pharmacology technique was used to connect these 242 targets. Comptotheca acuminata's interaction with colorectal cancer-related targets, overlapping targets imported into the STRING, human (homo sapiens) as the set condition, and a minimum interaction threshold of 0.4 utilised to build the PPI network. Cytoscape received the PPI network diagram. In order to create a PPI network,

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overlapping targets were imported into the STRING database (version 11.0) (Figure 3a). The minimum necessary interaction score was preset at medium confidence (>0.400) and the species was set to Homo sapiens., with other parameters kept as default. The (Figure 3b) MCL clustering 1 method was applied to identify functional modules within the network.

➢ *Target protein*

From the 3D structure of target Caspase 3, The PDB database provided the 3D structure of the protein; its PDB ID is 3DEI. The three-dimensional structure of the target protein is shown in Figure 2.

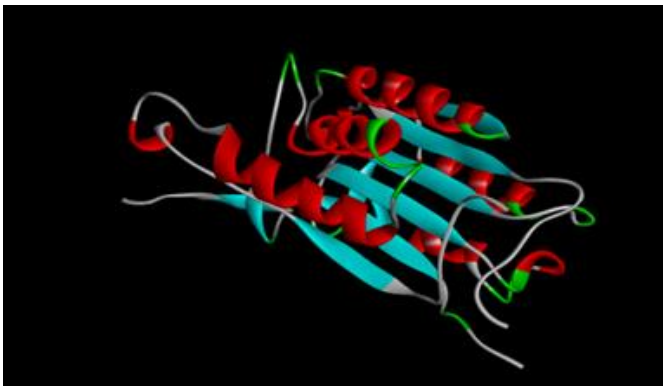

Fig 1 Overlapping Targets of CA Targets and CRC Targets

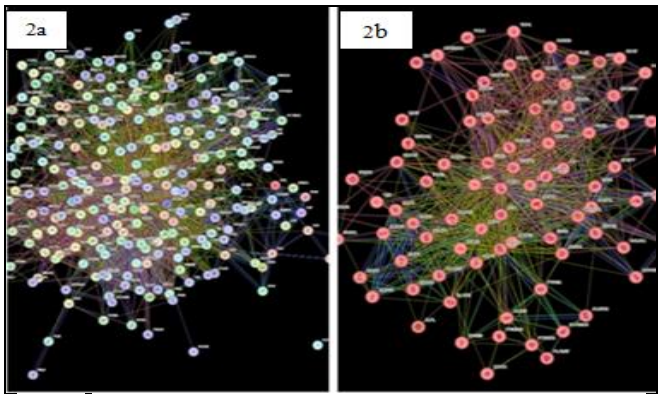

Fig 2a Protein - Protein Interaction of Overlapping Targets 2b: Protein - Protein Interaction of MCL Cluster 1 Functional Modules

The resulting MCL cluster interaction network data were downloaded in TSV format and imported into Cytoscape (3.9.1) after that. The top 10 hub proteins in the network depicted in (Figure 4b) were determined by calculating important topological metrics as degree centrality, betweenness centrality, and proximity centrality using Network Analyser.

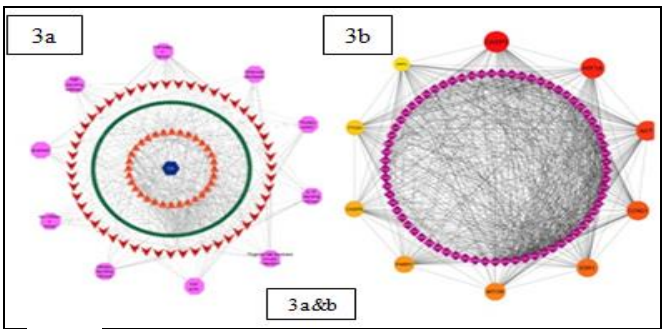

Fig 3a: CA-CRC-PATHWAYS Interaction of Functional Module 3b: Protein - Protein Interaction of Top 10 Hub Proteins MCL Cluster 1 Functional Module

Table 1 Interaction of Phytocompounds with the target Protein

S.NO	PUBCHEM ID	COMPOUNDS NAME
1.	24360	Camptothecin
2	97226	10-hydroxycamptothecin
3.	97283	10-methoxycamptothecin
4.	135515469	11-hydroxycamptothecin
5.	630607	11-methoxycamptothecin
6.	159549	18-hydroxycamptothecin
7.	9886692	O-Acetylcamptothecin
8.	9883320	22-hydroxyacuminatine
9.	3084765	Angustoline
10.	5320030	Naucleficine
11.	10163855	Vincosamide
12.	10345799	Strictosamide

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13.	5315179	Venoterpine
14.	85076	1,2-dihydro-2 oxoquinoline-4-carboxylic
15.	5280343	Quercetin
16.	64945	Ursolic acid
17.	160465	Bassic acid
18.	64971	9-Nitrocamptothecin
19.	177828320	Strychnolactone
20.	5280896	Abscisic acid
21.	89640	Loganic acid
22.	1794427	Chlorogenic Acid
23.	370	Gallic acid
24.	10742	Syringic acid
25.	338	Salicylic acid
26.	5317238	Ethyl caffeate
27.	15612	Dimethyl azelate
28.	161036	Sweroside
29.	100067	Syringaresinol
30.	2723872	Fructose
31.	5281860	3,7,8-Tri-O-methylellagic acid
32.	5491816	3,4'-Di-O-methylellagic acid

➢ *GO and KEGG Enrichment Analysis*

The enrichment analysis shows that Caspase-3 (CASP3) plays an important role in several cellular processes related to disease. It is involved in responses to chemical and oxidative stress, regulation of apoptosis, cell communication, and cell growth. CASP3 is mainly located in the plasma membrane, receptor complexes, and intracellular regions, indicating its role in signalling. It also shows functions such as protein kinase activity, ATP binding, and receptor activity. CASP3 is associated with major cancer-related pathways, including as the interleukin, TNF, Ras, MAPK, and PI3K-Akt signalling pathways. These pathways regulate cell survival and apoptosis, and their disruption may help cancer cells survive. Pathway enrichment analysis also shows that CASP3 is involved in processes related to tumour progression. The most enriched pathway is Angiogenesis, which supports tumour growth. Other important pathways include the AGE-RAGE signalling pathway and Endostatin M signalling pathway, indicating roles in inflammation and immune response. Overall, CASP3 is a key protein that regulates apoptosis and plays an important role in cancer development.

➢ *Molecular Docking*

Ligand–protein interactions may be involved in this application, as indicated by the observed binding affinities. Water molecules were removed during protein preparation. A molecular docking study was performed using 34 ligands and one receptor. Among these, 10 compounds showed the best docking results (Table 2). However synthetic drugs were also included in the analysis; however, they showed lower binding affinity compared with the selected compounds' Docking experiments for the phytocompounds (ligands) and the target CASP3 (PDB ID: 3DEI) protein for colorectal cancer were carried out using pyrx 0.8 software. The results showed that the majority of the compounds interacted with the target protein, and the following ten compounds had outstanding protein binding affinities. All the results are shown in Table 2, and the 2D and 3D interactions of phytocompounds with the target protein are shown in Figures 5 through 14.

Ten compounds, including compound 10-hydroxycamptothecin, shown excellent binding affinity (-8.1 Kcal/mol) with the target protein's amino acid residues LYS38, LYS154, TYR41, and SER109, according to the data (Table 2).The phytocompound Strictosamide also gave excellent binding affinity of -8.1 Kcal/mol with the amino acid residues PHE256, HIS121, TYR204, THR62 and ARG207. The binding affinity -8 Kcal/mol was observed between the phytocompound Vincosamide and the amino acid residues PHE256, TRP206, ASN208, SER249 of the target protein. The phytocompound camptothecin was found to have a binding affinity of -7.9 Kcal/mol with the target protein's amino acid residues LYS38, TYR41, LYS154, SER109, and SER154. The phytocompound 3,4'-Di-O-methylellagic acid showed the lowest binding affinity (-7.7 Kcal/mol) with the target protein's amino acid residues HIS121, ARG64, ALA162, ARG164, and GLU123. Additionally, the amino acid residues that interacted with the synthetic medication leucovorin were ARG207, SER205, GLY165, ARG164, GLY122, ALA162, GLN161, SER120, ARG64, and HIS121. The binding affinity of the drug with the target protein was -7.6 Kcal/mol. The amino acid residues that interacted with the synthetic medicine leucovorin were ARG207, SER205, GLY165, ARG164, GLY122, ALA162, GLN161, SER120, ARG64, and HIS121. The medication has a -7.6 Kcal/mol binding affinity with the target protein. When compared to the synthetic drug Leucovorin, the phytocompounds 10-hydroxycamptothecin, Strictosamide, Vincosamide, and Camptothecin demonstrated the highest binding affinity among the other phytocompounds in the current study. The binding affinity of the synthetic drug 5-Fluorourcil with the target protein was -4.9 Kcal/mol and the interacted amino acid residues were. Similarly, the phytocompounds 10-hydroxycamptothecin, Strictosamide, Vincosamide, and Camptothecin from Camptotheca Accuminata were found to have the potential to function as a medication for the treatment of colorectal cancer in the current in silico docking investigations.

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Tab 2 Interaction of Phytocompounds with the target protein

S.NO	PUBCHEM	COMPOUNDS NAME	BINDING AFFINITY	NO. OF BONDS	AMINO ACIDS RESIDUES	BOND LENGTH
1	97226	10-hydroxycamptothecin	-8.1	6	LYS38	4.6
					LYS154	5.12
					LYS154	5.19
					TYR41	2.89
					SER109	2.83
					SER109	2.67
2	10345799	Strictosamide	-8.1	9	PHE256	4.06
					PHE256	4.25
					PHE256	4.59
					HIS121	4.64
					TYR204	4.91
					THR62	2.73
					SER63	1.9
					SER63	2.63
					ARG207	2.21
3	10163855	Vincosamide	-8	7	PHE256	3.82
					PHE256	4.36
					PHE256	5.54
					TRP206	5.3
					ASN208	2.96
					ASN208	3.04
					SER249	3.54
4	24360	Camptothecin	-7.9	6	LYS38	4.64
					TYR41	2.9
					LYS154 LYS154	5.18
					SER109	5.11
					SER154	2.7
						2.64
5	3084765	Angustoline	-7.8	8	SER205	2.78
					GLY122	2.86
					HIS121	4.95
					HIS121	4.68
					THR166	3.78
					GLU123	3.62
					TYR204	5.27
					TYR204	3.68
6	9886692	O-Acetylcamptothecin	-7.8	6	SER65	2.9
					ARG207	3.08
					TRP206	5.88
					TRP206	5.25
					TYR204	3.84
					TYR204	3.32
7	64945	Ursolic acid	-7.7	2	GLY122	2.36
					TYR204	3.93

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8	160465	Bassic acid	-7.7	3	PHE250 ARG207 SER65	2.97 3.21 3.24
9	5320030	Naucleficine	-7.7	8	TYR204 TYR204 HIS121 HIS121 GLY122 GLY122 THR166 GLU123	3.93 4.57 5.25 5 2.65 3.19 3.72 3.62
10	5491816	3,4'-Di-O-methylellagic acid	-7.7	6	HIS121 HIS121 ARG64 ALA162 ARG164 GLU123	3.13 4.23 3.96 3.34 2.8 3.63
Synthetic drug						
11	135403648	leucovorin	-7.6	11	ARG207 ARG207 SER205 GLY165 ARG164 GLY122 ALA162 GLN161 SER120 ARG64 HIS121	2 2.04 2.94 2.33 2.43 2.19 3.79 2.68 2.58 1.38 2.33
12	3385	5-Fluorouracil	-4.9	8	TYR204 ARG207 ARG207 GLN161 ARG64 ALA162 SER120 HIS121	2.86 3.22 3.46 3.04 3.26 3.54 2.38 4.02

➢ *ADMET and CYP Properties*

The ADMET properties of the best-interacting phytocompounds and the synthetic drug Leucovorin, 5-Fluorourcil, were examined using SwissADME in the current study, and the findings were tabulated (table 3). The results show that all of the best-interacted phytocompounds, 5-fluorourcil, a synthetic drug, and leucovorin all adhere to the Lipinski rule of five. The majority of the drugs did not cross the blood-brain barrier (BBB) and showed high intestinal absorption (HIA). It is anticipated that P glycoprotein will eliminate many phytochemicals from the central nervous system. The XLogP3 readings of five of the ten compounds were within the permissible range. Every compound had rotatable bonds that fell within the allowed range. Naucleficine (PubChem CID: 5320030) and Angustoline were identified from the phytocompounds' Boiled Egg picture (Figure 15). (PubChem CID: 3084765) are in the egg yolk area, indicating that the substances can cross the blood-brain barrier and are passively absorbed by the digestive system. Additionally, the substances 10-hydroxycamptothecin (PubChem CID: 97226), Camptothecin (PubChem CID: 24360), O-Acetylcamptothecin (PubChem CID: 9886692), Bassic acid (PubChem CID: 160465), 3,4'-Di-O-methylellagic acid (PubChem CID: 5491816), and 5-Fluorouracil (PubChem CID: 3385) are found in the egg-white region. According to the results of CYP characteristics, the majority of the drugs do not inhibit the CYP450 enzymes or have any adverse side effects. The plant chemical Camptothecin blocks the CYP1A2, CYP2C9, CYP3A4, 10-hydroxycamptothecin blocks CYP1A2, O-Acetylcamptothecin blocks CYP2C19, CYP2C9, CYP3A4, Naucleficine blocks CYP1A2, and 3,4'-Di-O-methylellagic acid CYP1A2, CYP3A4 respectively. According to this statement, Phytocompounds Strictosamide, Vincosamide, Camptothecin, 10-hydroxycamptothecin, O-Acetylcamptothecin, Angustoline, 3,4'-Di-O-methylellagic acid permeation ability.

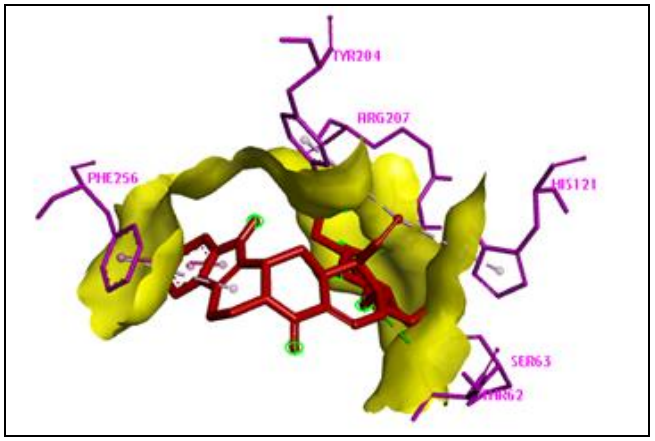

Fig 4 The 2D Interaction of Phytocompound 10-Hydroxycamptothecin with the Target Protein

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Tab 3 ADMET Properties of Phyto Compounds

S.No	PUBCHEM (CID)	COMPOUND NAME	LIPINSKI	BBB	HIA	PGP-	XLOG P3	TPSA(Å)	Log S (ESOL)	FRACTION Csp3	ROTATABLE BONDs
1	24360	Camptothecin	Yes	No	High	No	1.74	81.42	-3.49	0.25	1
2	97226	10-hydroxycamptothecin	Yes	No	High	No	1.38	101.65	-3.34	0.25	1
3	9886692	O-Acetylcamptothecin	Yes	No	High	Yes	2.31	87.49	-3.93	0.27	3
4	3084765	Angustoline	Yes	Yes	High	No	1.79	70.91	-3.52	0.2	1
5	5320030	Naucleficine	Yes	Yes	High	No	2.81	54.86	-4.08	0.1	1
6	10163855	Vincosamide	Yes	No	Low	No	0.41	144.71	-3.11	0.5	4
7	10345799	Strictosamide	Yes	No	Low	No	0.41	144.71	-3.11	0.5	4
8	64945	Ursolic acid	Yes	No	Low	Yes	7.34	57.53	-7.23	0.9	1
9	160465	Bassic acid	Yes	No	High	No	5.06	97.99	-5.91	0.83	2
10	5491816	3,4'-Di-O-methylellagic	Yes	No	High	Yes	1.76	119.34	-3.36	0.12	2
SYNTHETIC DRUG											
11	3385	5-Fluorouracil	Yes	No	High	Yes	-1.24	65.72	-0.58	0	0
12	135403648	leucovorin	No	No	Low	No	-0.89	219.84	-1.53	0.3	11

Tab 4 Cytochrome P450 Properties of Phytocompounds

S. NO	PUBCHEM (CID)	COMPOUND NAME	CYP1A2 Inhibitor	CYP2C19 Inhibitor	CYP2C9 Inhibitor	CYP2D6 Inhibitor	CYP3A4 Inhibitor	Log Kp (Skin Permeation)	A BIOAVAILABILITY SCORE (ABS)
1	24360	Camptothecin	Yes	No	Yes	No	Yes	-7.19	0.55
2	97226	10-hydroxycamptothecin	Yes	No	No	No	No	-7.54	0.55
3	9886692	O-Acetylcamptothecin	No	Yes	Yes	No	Yes	-7.04	0.55
4	3084765	Angustoline	Yes	No	No	Yes	No	-7.05	0.55
5	5320030	Naucleficine	Yes	No	No	No	No	-6.22	0.55
6	1E+07	Vincosamide	No	No	No	No	No	-9.05	0.56
7	1E+07	Strictosamide	No	No	No	No	No	-9.05	0.56
8	64945	Ursolic acid	No	No	No	No	No	-3.87	0.85
9	160465	Bassic acid	No	No	No	No	No	-5.68	0.56
10	5491816	3,4'-Di-O methylellagic acid	Yes	No	No	No	Yes	-7.06	0.55
SYNTHETIC DRUG									
11	3385	5-Fluorouracil	No	No	No	No	No	-7.73	0.55
22	1.4E+08	leucovorin	No	No	No	No	No	-10.07	0.11

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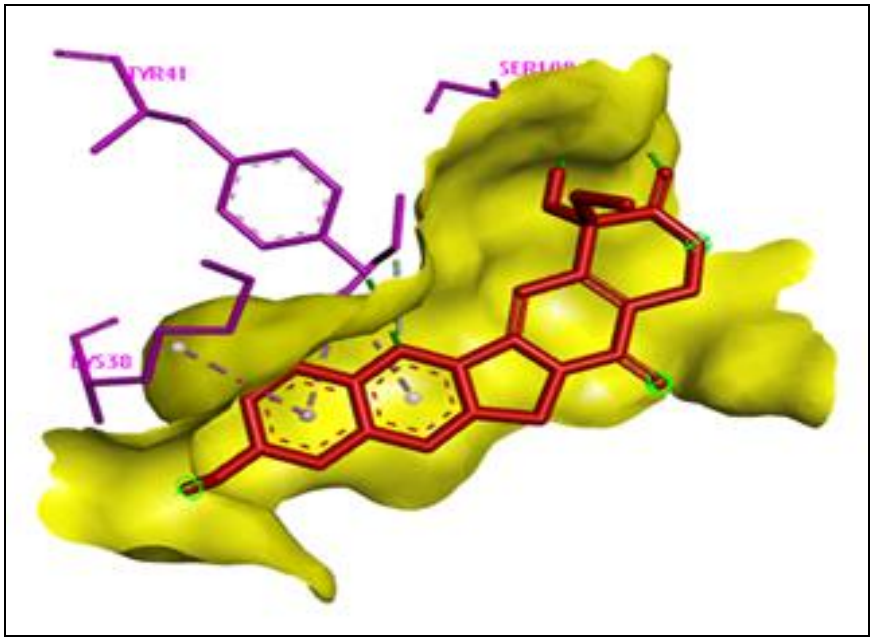

Fig 5 The 3D Interaction of Phytocompound 10-Hydroxycamptothecin with the Target Protein

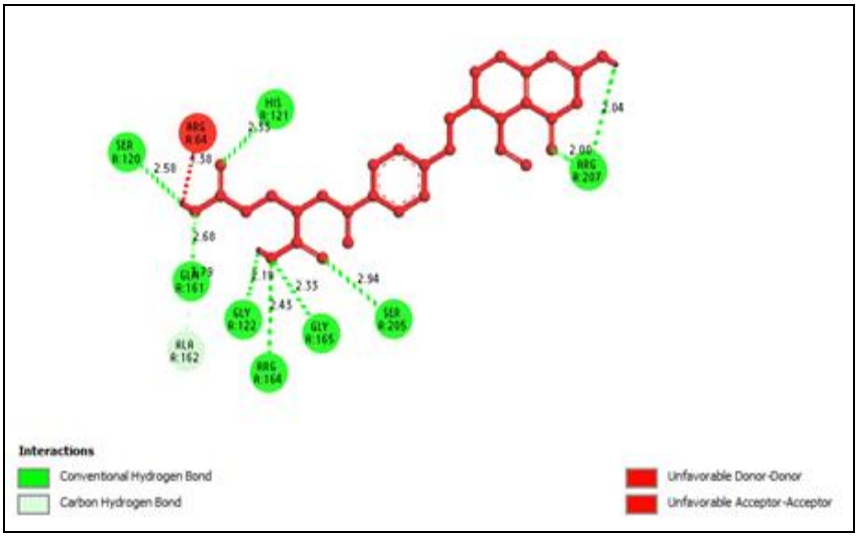

Fig 6 The 2D Interaction of Phytocompound Strictosamide with the Target Protein

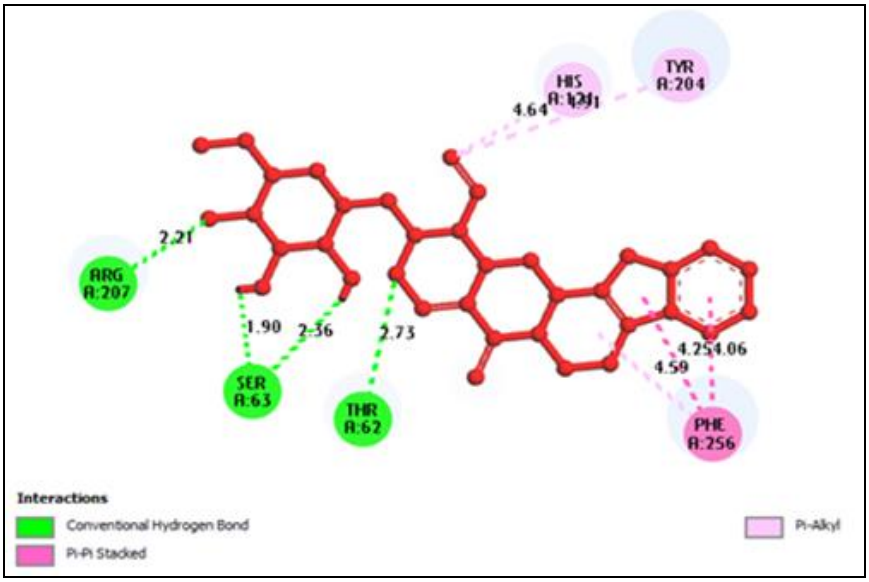

Fig 7 The 3D Interaction of Phytocompound Strictosamide with the Target Protein

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Certain molecules in the yolk of the BOILED-Egg are expected to passively cross the blood-brain barrier. It is believed that the gastrointestinal tract passively absorbs molecules known as HIA-Points found in the white of BOILED eggs. PGP+: Compounds that the P glycoprotein predicts will be removed from the central nervous system are indicated by blue dots. PGP-: Compounds that the P glycoprotein predicts won't be removed from the central nervous system are indicated by red dots.

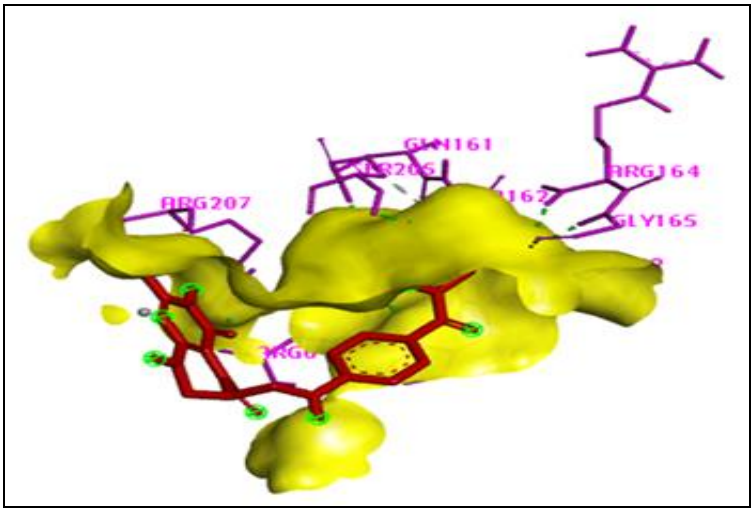

Fig 8 The 2D Interaction of Phytocompound Vincosamide with the Target Protein

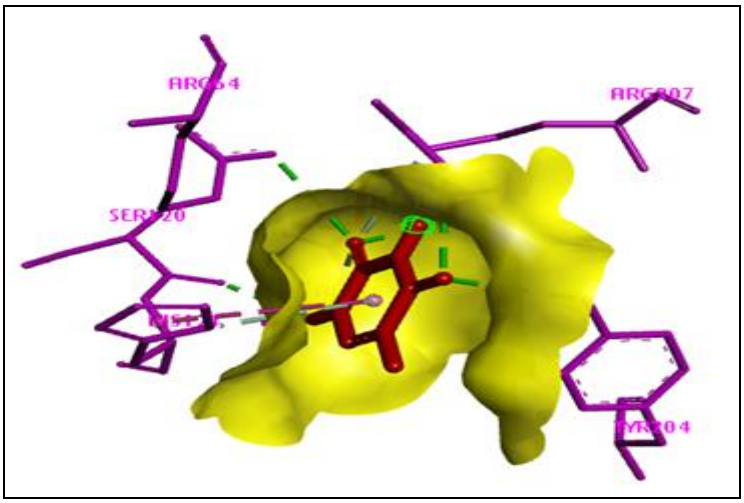

Fig 9 The 3D Interaction of Phytocompound Vincosamide with the Target Protein

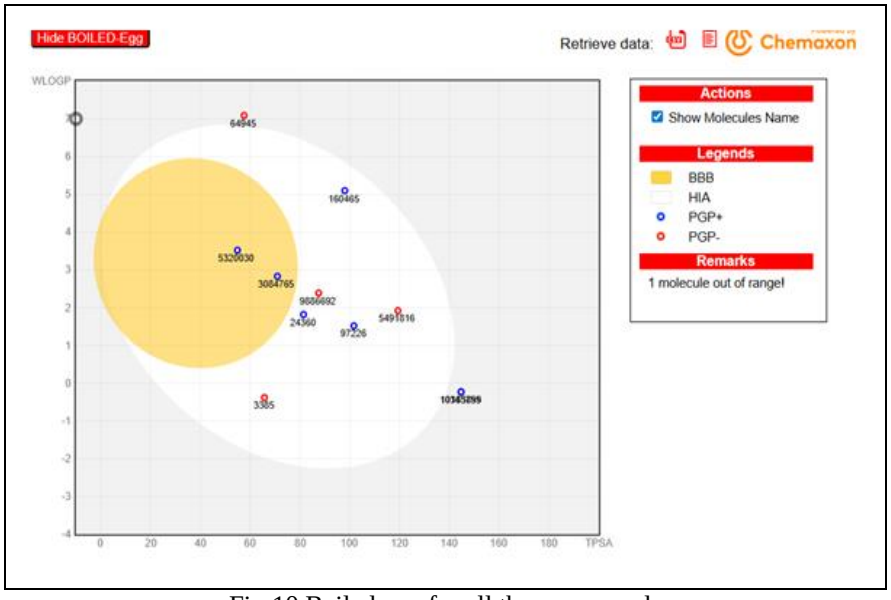

Fig 10 Boiled egg for all the compounds

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IV. DISCUSSIONS

Plant-derived chemicals, especially those generated from Camptotheca acuminata, are becoming increasingly important in cancer research, according to recent studies. The de novo genome assembly of Camptotheca acuminata was described by Zhao et al. (2017), which revealed important genes involved in camptothecin production and offered a solid basis for the creation of anticancer drugs.In a similar situation, Mahdi *et al.* (2025) investigated camptothecin derivatives using molecular docking and dynamics simulations, revealing stable interactions with cancer-related proteins and highlighting their potential as effective therapeutic agents. Network pharmacology approaches have further emphasized the multi-target nature of natural compounds. He *et al.* (2023) demonstrated the therapeutic potential of curcumin in colon cancer by identifying multiple targets and pathways. While Huang *et al.* (2020) reported that traditional formulations such as Zuojinwan exhibit multi-component and multi-target mechanisms against colorectal cancer. In agreement with these findings, the present study identified key targets such as Caspase-3 (CASP3) and TP53, which are essential regulators of apoptosis and tumour progression. Furthermore, Adak *et al.* (2024) highlighted the integration of phytocompounds with nanotechnology for improved targeting and reduced toxicity, whereas Isa *et al.* (2024) demonstrated the effectiveness of combining molecular docking, ADME analysis, and molecular dynamics simulations in identifying promising anticancer compounds. Consistent with these studies, the present work revealed that compounds derived from Camptotheca acuminata exhibit strong binding affinity toward key colorectal cancer targets, along with favourable pharmacokinetic properties and reduced toxicity when compared to conventional chemotherapy drugs.

Overall, the results lend credence to the idea that chemicals derived from plants function via several targets and pathways, providing a potentially effective therapy approach for colorectal cancer. To establish their clinical promise, however, more experimental validation through in vitro and in vivo research is needed.

REFERENCES

[1]. Adak, D., Ray, P., & Setua, S. (2024). Unlocking therapeutic precision: "Camptotheca acuminata, a traditional Chinese herb tailored for phytonano-cancer theranostics". *Pharmacological Research-Modern Chinese Medicine*, *11*, 100447

[2]. Balata, G. F., & Azzam, H. N. (2025). Synopsis of colorectal cancer: prevalence, symptoms, screening, staging, risk factors, and treatment. *The Egyptian Journal of Internal Medicine*, *37*(1), 4.

[3]. De, S.; Paul, S.; Manna, A.; Majumder, C.; Pal, K.; Casarcia, N.; Mondal, A.; Banerjee, S.; Nelson, V.K.; Ghosh, S.; et al. Phenolic Phytochemicals for Prevention and Treatment of Colorectal Cancer: A Critical Evaluation of In Vivo Studies. Cancers 2023, 15, 993. https:// doi.org/10.3390/cancers15030993

[4]. Gurjar, S. P., Roy, A., & Gupta, A. (2024). Analysis of Phytochemicals from Camptotheca acuminata, Curcuma longa, and Diphylleia grayi Against a Complex of ERK2 with Catechol. *Letters in applied nanobioscience*, *13*(3), 141.

[5]. He Q, Liu C, Wang X, Rong K, Zhu M, Duan L, Zheng P and Mi Y (2023) Exploring the mechanism of curcumin in the treatment of colon cancer based on network pharmacology and molecular docking. Front. Pharmacol. 14:1102581. doi: 10.3389/fphar.2023.1102581

[6]. Isa, A. S., Uzairu, A., Umar, U. M., Ibrahim, M. T., Umar, A. B., & Ahmad, I. (2024). Potential anti-colon cancer agents: Molecular modelling, docking, pharmacokinetics studies and molecular dynamic simulations. *Journal of Holistic Integrative Pharmacy*, *5*(3), 235-247.

[7]. Jagtap, N., Singh, A. P., Inavolu, P., Tandan, M., Godbole, S., Ambardekar, P., ... & Reddy, D. N. (2021). Detection of colon polyps in India—a large retrospective cohort studies (DoCPIr). *Journal of Digestive Endoscopy*, *12*(02), 063-066.

[8]. Kee, J. X., Yau, J. N. N., Kumar Muthuramalingam, R. P., Wang, X., Chng, W. H., Lopez-Sanchez, A., ... & Pastorin, G. (2025). Colorectal cancer at the crossroads: the good, the bad, and the future of platinum-based drugs. *Chemical Reviews*, *125*(21), 10248-10341.

[9]. Li, S., & Wang, P. (2014). Phytochemistry of Camptotheca decaisne.

[10]. Mahdi, Z. A. A., Almjalawi, B. S. A., Naimuzzaman, M., Hasan, M., Al-Alaq, F. T., Al-Dahmoshi, H. O., ... & Saki, M. (2025). Exploring Camptothecin Derivatives from the Chinese Tree of Camptotheca acuminata as Breast Cancer Protease Inhibitors: Insights from Multi-Scale Computational Analysis. *The Open Bioinformatics Journal*, *18*(1).

[11]. Siqi Huang, Zheyu Zhang, Wenqun Li, Fanhua Kong, Pengji Yi, Jianhua Huang, Dan Mao, Weijun Peng & Sifang Zhang (2020) Network Pharmacology-Based Prediction and Verification of the Active Ingredients and Potential Targets of Zuojinwan for Treating Colorectal Cancer, Drug Design, Development and Therapy, 2725-2740, DOI: 10.2147/ DDDT.S250991

[12]. Shivshankar, S., Patil, P. S., Deodhar, K., & Budukh, A. M. (2025). Epidemiology of colorectal cancer: A review with special emphasis on India. *Indian Journal of Gastroenterology*, *44*(2), 142-153.

[13]. Yang, Z., Deng, X., Yang, Z., Han, M., Zanna, M. Y., Ismail, N., ... & Chan, K. W. (2025). Current chemotherapy strategies for colorectal cancer: challenges and future directions. *Asian Journal of Medicine and Biomedicine*, *9*(1), 59-86.

[14]. Zhao, D., Hamilton, J. P., Pham, G. M., Crisovan, E., Wiegert-Rininger, K., Vaillancourt, B., ... & Buell, C. R. (2017). De novo genome assembly of Camptotheca acuminata, a natural source of the anti-cancer compound camptothecin. *GigaScience*, *6*(9), gix065.