ISSN 0974-3618 (Print)
0974-360X (Online)
www.rjptonline.org

RESEARCH ARTICLE

In-Silico Approach Based Identification of Potential Bioactive Compounds from Phytochemicals as Inhibitors of Hbv- Mediated Hepatocellular Carcinoma

P.R.Kiresee Saghana[1]*, S. Shanmugavani[2], R. Priya[2], P. Amudha[3] and V.Dhivya[4]

[1]Assistant Professor Department of Bioinformatics, School of Life Sciences, Vels Institute of Science, Technology and Advanced Studies (VISTAS), Pallavaram, Chennai-600117, Tamil Nadu, India.

[2]Assistant Professor Department of Bioinformatics, School of Life Sciences, Vels Institute of Science, Technology and Advanced Studies (VISTAS), Pallavaram, Chennai-600117, Tamil Nadu, India.

[3]Assistant Professor Department of Biochemistry, School of Life Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram, Chennai - 600117, Tamil Nadu, India.

[4]Assistant Professor Department of Civil Engineering, Vels Institute of Science and Technology in Advanced Studies (VISTAS), Pallavaram, Chennai-600117, Tamil Nadu, India.

*Corresponding Author E-mail: **kireseesaghana.sls@velsuniv.ac.in**

ABSTRACT:

Hepatocellular carcinoma (HCC) is the most prevalent form of liver cancer, representing approximately 90% of all liver cancer cases and is the second leading cause of cancer-related deaths. Hepatitis B virus (HBV) infection is the primary risk factor for HCC, responsible for about 70-80% of HCC cases in India and around 55% worldwide. This study aims to identify bioactive compounds that can counteract Hepatitis B infection. The human hepatitis B capsid protein (1QGT), a key protein involved in the malignant transformation process, was selected for virtual screening with various phytochemical compounds from different plants. Following virtual screening and pharmacokinetic analysis using Swiss ADME and admetSAR, 16 compounds were shortlisted and docked with the target protein using AutoDock Vina. The docking results were compared to Tenofovir. The analysis indicated that the compounds 4,7-Methanofuro[3,2-c] oxacycloundecin-6(4H) one (-8.7kcal/mol) and Luvangetin (-8.1kcal/mol) are potential inhibitors of the Human Hepatitis B viral capsid protein.

KEYWORDS: Hepatocellular carcinoma, Hepatitis B infection, Hepatitis B capsid protein, virtual screening, docking.

INTRODUCTION:

Hepatocellular carcinoma ranks as the fifth most common cancer and the fourth leading cause of cancer-related deaths globally. In men, it is the fourth most common malignant and the second leading cause of cancer-related deaths. Men have a higher risk of developing liver cancer compared to women. It is more prevalent in sub-Saharan Africa, East Asia, and Southeast Asia than in Western countries[1]. The 5-year survival rate for liver cancer ranges from only 5-30% (IARC and WHO, 2022). Secondary liver cancer occurs when cancer cells from another part of the body migrate to the liver. Cancers such as those in the breast, esophagus, stomach, pancreas, lungs, and kidneys can spread to the liver, but most secondary liver cancers come from colorectal cancer, with about 70% of

Received on 22.01.2025 Revised on 12.05.2025
Accepted on 01.07.2025 Published on 16.03.2026
Available online from March 18, 2026
Research J. Pharmacy and Technology. 2026;19(3):1357-1364.
DOI: 10.52711/0974-360X.2026.00195

colorectal cancer patients developing these tumors. Primary liver cancers include hepatocellular carcinoma (HCC) and intrahepatic cholangiocarcinoma (ICC), as well as rarer types like angiosarcoma, hemangiosarcoma, and hepatoblastoma. HCC arises from liver cells called hepatocytes, while ICC develops in the bile ducts.

Hepatitis B virus (HBV) is pivotal in initiating hepatocellular carcinoma (HCC). As a small DNA virus from the hepadnaviridae family, the infectious virion, termed the Dane particle, has a spherical, double-layered structure with a 42 nm diameter. Its outer lipid envelope contains viral surface antigens (HBsAg) facilitating viral binding and entry into host cells, enclosing an icosahedral nucleocapsid of core antigens (HBcAg). The nucleocapsid's single polypeptide chain, the core antigen HBcAg, weighs 20 kDa. The HBV capsid protein structure (PDB ID: 1QGT) is characterized by a long α-helical hairpin formed by residues 50–73 (α3) and 79–110 (α4), with a bend in the α4 helix between residues 90 and 92, separating it from the α3 helix. This protein is a promising target for HCC treatment.

Indian medicinal flora is abundant in pharmacologically active ingredients, commonly used in traditional remedies for various conditions. Secondary metabolites from these plants, including alkaloids, tannins, steroids, terpenoids, coumarins, and phenolic compounds, are significant in anticancer drug therapy. Thus, this study aimed to evaluate the in silico inhibitory potential of 175 major phytocompounds from seven different medicinal plants: roots of Circhorium intybus, Curcuma angustifolia, leaves of Amaranthus spinosus, Centella asiatica, Corchorus aestuans, Andrographis paniculata, and fruit of Aegle marmelos, retrieved from the PubChem database. The phytocompounds identified through in silico studies could pave the way for in vitro testing and clinical trials, potentially accelerating drug discovery for liver cancer. To our knowledge, no previous studies have been conducted in this area. This proposed study is novel and holds significant potential in cancer research.

MATERIALS AND METHODS:

Target selection

The core protein (Cp) of the Hepatitis B viral capsid plays vital roles in the virus's life cycle and is implicated in the process of malignant transformation that results in Hepatocellular carcinoma. The three-dimensional crystal structure of this target protein is obtained from the RCSB database in .pdb format[6]. (www.rcsb.org).

Compounds collection

The selected plants are Circhorium intybus, Amaranthus spinosus, Centella asiatica, Corchorus aestuans, Andrographis paniculata, Curcuma angustifolia and Aegle marmelos. The compounds derived from these plants are obtained from the PubChem database in .sdf format (https://pubchem.ncbi.nlm.nih.gov/). Subsequently, these compounds are utilized for virtual screening[7].

Virtual screening

PyRx is a virtual screening software utilized in computational drug discovery. It screens a library of phytochemical compounds against a target protein. PyRx allows medicinal chemists to perform virtual screening from any platform and assists users throughout the process. The selected target protein is prepared as a macromolecule and converted to the .pdbqt format. The selected compounds are designated as ligands and also converted to the .pdbqt format. Subsequent energy minimization steps are then carried out. The selection of small molecules is based on the binding energy results from the virtual screening.[8]

ADME property prediction

In this context, we specifically check the carcinogenicity property of the compounds. Additionally, since the SDF file format is not compatible with Autodock tools 1.5.7, the selected compounds' file format is converted from SDF to PDB using BIOVA Discovery Studio[9].

Autodock vina:

AutoDockVina.(URL: vina.scripps.edu). The protein and ligand pdb files are uploaded in autodock tools and then they converted to pdbqt formats further they are run in the command prompt for the docking results. We get a log file as a text document and the output file in pdbqt format.

BIOVA Discovery studio visualization for ligand interactions:

It is used to analyze the protein-ligand interactions, create 2D interaction plots, heat maps, and 3D point plots and so on. It was downloaded from the URL:https://discover.3ds.com/discovery-studio-visualizer-down

RESULTS AND DISSCUSSION:

This research focused on analyzing the binding of diverse phytochemicals to the hepatitis B capsid protein (1QGT), a target connected to liver cancer, through computational docking techniques. A total of 175 phytochemicals were chosen for their potential to inhibit proteins associated with HCC. These compounds, sourced from the PDB database, are illustrated in Figure 1. The selection includes organic molecules like fatty acids, carbohydrates, benzene derivatives, chromones, polyphenols, and amino acids.[10,21]

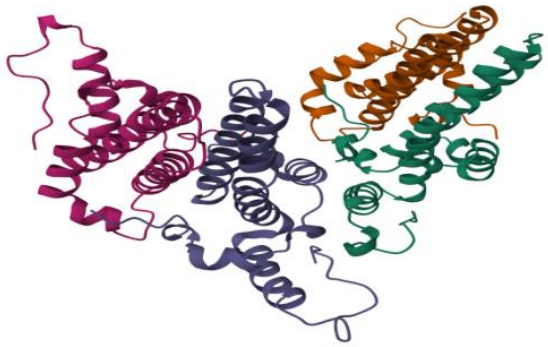


Figure 1. 3D structure of the core protein

COMPOUNDS COLLECTION

The drug-likeness of the studied phytochemicals was evaluated using Lipinski's rule of five. This rule was applied to 175 phytochemicals with high binding affinity to the selected proteins[11,22]. Any compounds violating one or more of Lipinski's rules were excluded, and the remaining ones were further examined for toxicity. Additionally, hydrogen bonds are crucial in drug design as they play a significant role in drug permeation, metabolism, and absorption. Compounds from seven different plants were obtained from the PubChem database in sdf format. Table 2 presents the number of compounds retrieved from each plant[12].

Table.2 Compounds collection

PLANTS	NO. OF COMPOUNDS
Circhorium intybus	49
Amaranthus spinosus	23
Centella asiatica	31
Corchorus aestuans	12
Andrographis paniculata	11
Curcuma angustifolia	32
Aegle marmelos	17
Total	**175**

VIRTUAL SCREENING

The molecular docking method seeks to determine the correct positioning of the ligand within binding proteins and to predict affinity between the target and the ligand. PyRx software, utilizing the Autodock Vina virtual screening tool[14,20], was employed for the docking process and to visualize 2D patterns of ligand-target protein interactions. The top drug candidates were identified based on their binding affinities.[13] PyRx revealed the occupancy of the ligand in the target molecule's binding pocket through conformation scores. The virtual screening was performed using the conjugate gradient method of energy minimization with the UFF force field. We selected compounds with binding affinities less than -7.5, resulting in 32 compounds listed in Tables 3 and 4.

Table 3. Binding energy results

S.NO	COMPOUND NAME	BINDING AFFINITY (kcal/mol)
1	Alantolactone	-10.4
2	Vitamin E	-10.3
3	Ledene oxide 1	-10.3
4	Taraxasterol	-9.8
5	Gamma tocopherol	-9.5
6	Beta elemene	-9.4
7	Campersterol	-9.3
8	Cyclohexane	-9.3
9	Gamma elemene	-9.3
10	Lupeol	-9.2
11	Stigmasterol	-8.9
12	Trioxsalen	-8.9
13	4,7-Methanofuro[3,2-c] oxacycloundecin-6(4H)-one	-8.9
14	Marmin	-8.8
15	Marmesinin	-8.6
16	Marmelosin	-8.6
17	1-H-Cycloprop[e]azulene	-8.6
18	4-[(2,6-dichlorobenzyl)oxy]-3-ethoxybenzaldehyde	-8.3
19	Beta sitosterol	-8.3
20	5-formyl-2furyl methyl acetate	-8.3
21	Curzerene	-8.1
22	Aegeline	-8.1
23	(+)-Norreticuline	-8.0
24	Stigmast-5-en-3-ol	-7.9
25	Undec-3-en-2-ol	-7.9
26	Luvangetin	-8.1
27	Gamma-Fagarine	-7.8
28	Chlolesta-4,6-dien-3-ol	-7.7
29	(-)-Spathulenol	-7.7
30	Caryophyllene oxide	-7.6
31	Boreneol	-7.5
32	Naphtho[2,3-b] furan-2(3H)-one	-7.5

Table.4 :No. of compounds selected from each plant from binding energy results

Circhorium intybus	5
Amaranthus spinosus	3
Centella asiatica	6
Corchorus aestuans	1
Andrographis paniculata	0
Curcuma angustifolia	9
Aegle marmelos	7
Total	32

ADME PROPERTIES PREDICTIONS:

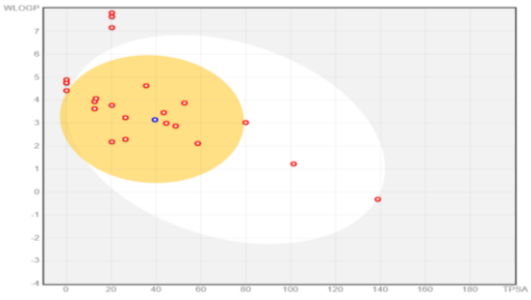


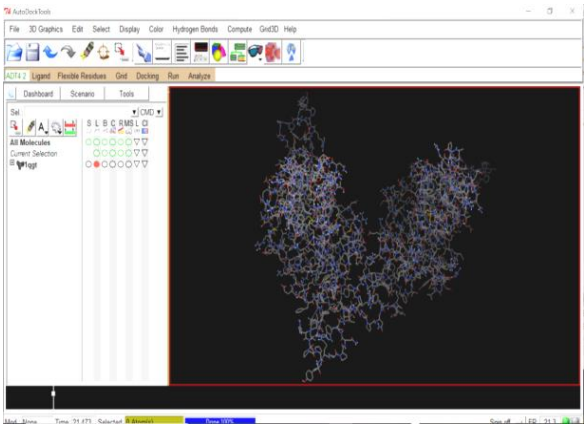
Figure 2. Boiled egg result from SWISS-ADME

Table 5. ADMET properties results from Swiss ADME and admetSAR

S. No	Plants	Compound name	MW	HBA	HBD	GI abs	RO5	GHOSE	Carcinogenicity
1	Circhorium intybus	Alantolactone	232.32	2	0	High	yes(0)	**yes**	Non- carcinogen
		4-[(2,6 dichlorobenzyl)oxy]-3-ethoxybenzaldehyde	325.19	3	0	High	yes (0)	yes	Non-carginogen
		undec-3-en-3-ol	222.37	1	1	High	yes(0)	**yes**	Non- carcinogen
2	Amaranthus spinosus	Ledene oxide I	220.35	1	0	High	yes(0)	**yes**	Non- carcinogen
		Boreneol	154.25	1	1	High	yes(0)	No	Non- carcinogen
3	Centella asiatica	(+)-Norreticuline	315.36	5	3	High	yes(0)	yes	Non- carcinogen
4	Curcuma angustifolia	Trioxsalen	228.24	3	0	High	yes(0)	yes	Non- carcinogen
		4,7-Methanofuro[3,2-c] oxacycloundecin-6(4H)-one	246.30	3	0	High	yes(0)	yes	Non- carcinogen
		Naphtho[2,3-b]furan-2(3H)-one	184.19	2	0	High	yes(0)	yes	Non- carcinogen
		Caryophyllene oxide	220.35	1	1	High	yes(0)	yes	Non- carcinogen
		Curzerene	216.32	1	0	High	yes(0)	yes	Non- carcinogen
		(-)-Spathulenol	220.35	1	1	High	yes(0)	yes	Non- carcinogen
5	Aegle marmelos	Marmelosin	270.28	4	0	High	yes(0)	yes	Non- carcinogen
		Luvangetin	258.27	4	0	High	yes(0)	yes	Non- carcinogen
		gamma-Fagarine	229.23	4	0	High	yes(0)	yes	Non- carcinogen
		Aegeline	297.35	3	2	High	yes(0)	yes	Non- carcinogen

DOCKING:

AutoDock Vina is utilized for drug discovery. Molecules are loaded, and water molecules are removed from the target protein structure. Polar hydrogens are added, along with Kollman charges. The protein is then saved in PDBQT format. Next, the ligand molecule is loaded and also saved in PDBQT format. The protein molecule is prepared, and a grid box is set with x, y, and z dimensions. The grid box dimensions are set to default. This grid box data is stored in a text file named `config.txt`, which is subsequently used for docking in the command prompt[15,19].



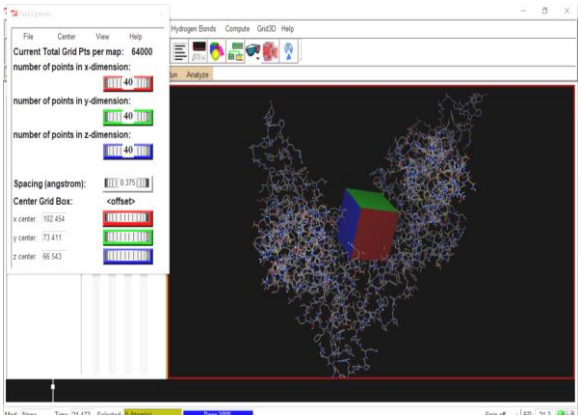


Figure 3. Grid box forming

EXECUTING THE DOCK IN THE COMMAND PROMPT

The docking process was executed via the command prompt using the grid center value, which was specified in the configuration file. This file was set up to allow only changes to the ligand name and output file name for each docking instance.[17,23] In the command prompt, the protein pdbqt file, ligand pdbqt file, configuration text document, and the vina application were executed. The results included a log file with binding affinity data and an output file in pdbqt format. This procedure was repeated for all 16 compounds with the target protein, yielding 16 output and log files. One control, named

tenofovir (currently used for chronic hepatitis B patients), was obtained from the Drug Bank.[18] Docking was conducted with tenofovir and the target protein, and the results were compared with the binding affinity and interactions of the other docked compounds. Ligands with better binding affinity and interactions than the control tenofovir are considered potential lead bioactive molecules against HBV-mediated hepatocellular carcinoma.

DISCOVERY STUDIO VISUALIZER:

The interactions between the target protein and the ligands were observed using BIOVIA Discovery Studio Visualizer, noting both 2D and 3D interactions. Table 6 presents the results.

Table 6. Docking results with interactions

S. NO	COMPOUND NAME	BINDING AFFINITY (kcal/mol)	INTERACTIONS		BOND LENGTH (in Å)
1	Alantolactone	-8.6	Hydrogen bonds	TYR 6	2.07
			Alkyl	CYS 61	5.20
				LEU 60	5.37
2	4-[(2,6-Dichlorobenzyl)oxy]-3-ethoxybenzaldehyde	-7.9	Carbon hydrogen bond	GLN 57	3.45
			Alkyl	LEU 60	5.06
			Pi-Alkyl	LEU 100	5.38
				LEU 60	4.72
				VAL 13	5.49
				LYS 96	4.06
				PRO 5	4.71
			Pi-Sulfur	CYS 61	-
3	undec-3-en-2-ol	-8.1	Hydrogen bond	TYR 6	2.68
			Alkyl	PRO 5	4.07
				LYS 96	4.09
				VAL 13	4.54
4	Ledene oxide I	-7.8	Alkyl	LEU 60	5.00,5.17
				LYS 96	4.61
				PRO 5	4.61,4.41
				LEU 100	4.49
5	Borneol	-6.5	Hydrogen bond	SER 106	2.50
			Alkyl	VAL 124	5.22
				LEU 30	5.03
				PRO 25	4.80
6	(+)-Norreticuline	-7.9	Hydrogen bond	CYS 61	2.93
			Carbon hydrogen bond	CYS 61	3.32
				GLN 57	3.56
				GLU 64	3.51
			Pi-sulfur	CYS 61	
			Alkyl	CYS 61	4.11
				ALA 58	4.37
				CYS 96	4.24
				LEU 95	5.46
			Pi-alkyl	LYS 96	3.74
				PRO 5	5.18
				VAL 13	5.04
7	Trioxsalen	-7.9	Hydrogen bond	LYS 96	3.08
			Alkyl	CYS 61	3.65,4.96
			Pi-alkyl	PRO 5	4.89,4.93
				LEU 60	4.85,4.70
				CYS 61	5.29
10	Caryophyllene oxide	-7.7	Alkyl	LYS 96	4.52
				PRO 5	4.44
				LEU 60	5.30
11	Curzerene	-7.6	Hydrogen bond	TYR 6	2.69
			Alkyl	VAL 13	3.90
				ILE 97	5.15
				LEU 100	4.60
			Pi-alkyl	LYS 96	4.24
				PRO 5	4.59
				VAL 13	5.23

12	(-)-Spathulenol	-8.1	Alkyl	LYS 96	4.01,4.49
				PRO 5	5.17,4.39
				LEU 100	4.41
13	Marmelosin	-7.6	Pi-Sigma	LEU 100	4.00
			Pi-Pi-T-shaped	TYR 6	5.27
			Pi- Alkyl	LYS 96	4.15,4.56
				PRO 5	4.60,4.72
				CYS 61	5.43
				LEU 100	5.15,4.47
14	Luvangetin	-8.1	Carbon hydrogen bond	LEU 60	3.49
				GLU 64	3.10
			Alkyl	LEU 60	4.01
				LEU 100	4.53
				ILE 97	5.41
				LYS 96	4.61
			Pi-alkyl	VAL 13	5.14
				LYS 96	4.44
				LEU 60	5.46
				PRO 5	4.33,3.93
15	Gamma-Fagarine	-7.2	Carbon hydrogen bond	GLN 99	3.42
			Pi-Sigma	LYS 96	3.90
			Pi-Sulfur	CYS 61	
16	Aegeline	-7.6	Hydrogen bond	TYR 6	1.91
			Carbon hydrogen bond	GLN 57	3.52
			Pi-Sigma	LEU 100	3.62
			Alkyl	CYS 61	4.32,4.65
				LEU 60	5.05
			Pi-Alkyl	LYS 96	5.16
				PRO 5	4.30

After the protein-ligand docking, the binding affinity of (+)-Norreticuline was found to be -7.9 kcal/mol, represented in a histogram format. This format illustrates various interactions: hydrogen bonding with CYS 61 (bond length 2.93 Å), three carbon-hydrogen bonds involving CYS 61, GLN 57, and GLU 64 (bond lengths 3.32, 3.56, and 3.51 Å respectively), a Pi-sulfur bond with CYS 61, and four alkyl bonds with CYS 61, ALA 58, CYS 96, and LEU 95 (bond lengths 4.11, 4.37, 4.24, and 5.46 Å respectively). Additionally, Pi-alkyl interactions were observed with LYS 96, PRO 5, and VAL 13, with bond angles of 3.74, 5.18, and 5.04 respectively.

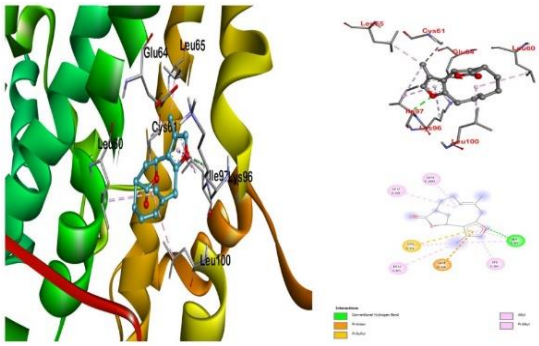


Figure 4. 3D and 2D interactions between 1QGT protein and 4,7-Methanofuro [3,2- c] oxacycloundecin-6(4H)-one

The Hepatitis B capsid protein interacts with 4,7-Methanofuro[3,2-c]oxacycloundecin-6(4H)-one with a binding affinity of -8.7 kcal/mol. It forms a hydrogen bond with ILE 97 at a bond length of 4.81 Å, along with alkyl and pi-alkyl interactions. Additionally, it engages in five alkyl bond interactions with LEU 100, LEU 60, LYS 61, LEU 65, and ILE 97, with bond lengths of 5.25, 3.90, 3.99, and 4.95 Å, respectively.

Table 6. Drug interactions with receptor

DRUG	BINDING AFFINITY (kcal/mol)	INTERACTIONS		BOND LENGTH (in Å)
Tenofovir	-6.7	Hydrogen bond	TYR 6, GLN 99, GLN 57	2.09, 1.99, 2.56
		Pi-Alkyl	VAL 13, LYS 96, PRO 5, LEU 100	4.56,3.96 ,5.01,4.26

The Hepatitis B capsid protein interacts with Luvangetin with a binding affinity of -8.1 kcal/mol. It demonstrates two carbon-hydrogen bond interactions with LEU 60 and GLU 64, with bond lengths of 3.49 and 3.10 Å, respectively, along with alkyl and pi-alkyl interactions involving four bonds.

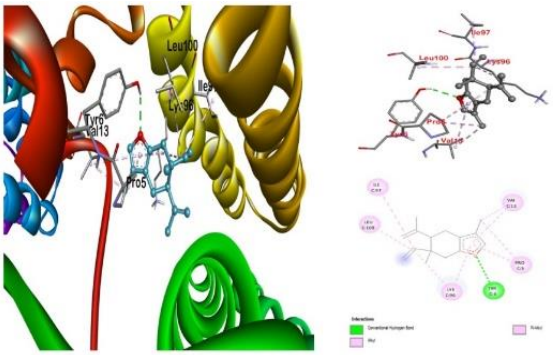


Figure 5. 3D and 2D interactions between 1QGT protein and Luvangetin

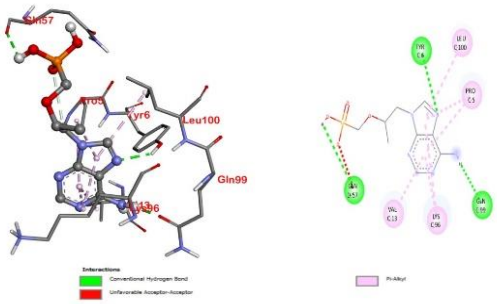


Figure 6. 3D and 2D interactions between 1QGT protein and Tenofovir(drug)

CONCLUSION:

Phytochemicals offer promising therapeutic potential due to their anti-inflammatory, antioxidative, anticholinesterase, and anticancer properties.While synthetic drugs may exhibit greater potency, they also carry unpredictable and hazardous risks compared to many illicit substances. Phytochemicals are increasingly recognized as a valuable source of effective yet safer agents against various life-threatening diseases. From the docking results, compounds like 4,7-Methanofuro[3,2-c]oxacycloundecin-6(4H)-one and Luvangetin are selected. The former, along with Curzerene from Curcuma angustifolia, demonstrates anti-inflammatory properties, while Luvangetin, Gamma-Fagarine, and Aegeline from Aegle marmelos exhibit anti-inflammatory, anti-HCV, and antiadipogenic activities. These six compounds exhibit superior binding affinities and interactions compared to the drug Tenofovir. Analysis of the docking results identifies 4,7-Methanofuro[3,2-c]oxacycloundecin-6(4H)-one and Luvangetin as potential inhibitors of the Hepatitis B viral capsid protein (1QGT). Further in vitro and in vivo analyses are strongly recommended for these compounds.

REFERENCES:

1. Acharya SK. Epidemiology of hepatocellular carcinoma in India. J Clin Exp Hepatol. 2014; 4(Suppl 3): S27–S33.
2. Albuquerque TAF, Drummond do Val L, Doherty A. From humans to hydra: Patterns of cancer across the tree of life. Biol Rev Camb Philos Soc. 2018; 93:1715-1734
3. Alcazar MA, Wright K, Vaswani A, Caruso, M, Reed RL, Bailey CF, Maier, CS. Integration of mass spectral fingerprinting analysis with precursor ion (MS1) quantification for the characterization of botanical extracts: application to extracts of Centella asiatica (L.) Urban. Phytochem Anal. 2020; 1-17.
4. Andrea Marengo, Chiara Rosso, and Elisabetta Bugianesi. Liver Cancer: Connections with Obesity, Fatty Liver, and Cirrhosis. ARI. 2015; 14: 14:13.
5. Anshid Venthodika, Navnidhi Chhikara, Sandeep Mann, Mukesh Kumar Garg, Sajad Ahmad Sofi, Anil Panghal. Bioactive compounds of Aegle marmelos L., medicinal values and its food applications: A critical review, John Wiley & Sons Ltd. 2020: 1–21.
6. Bajpai V. The challenges confronting public hospitals in India, their origins, and possible solutions. Adv Public Health. 2014; 2014: 898502.
7. Bo J, Li S, Ma P, Zhu Y, Zhang Y. Research on early warning mechanism and model of liver cancer rehabilitation based on CSSVM Hindawi. J Healthc Eng. 2021.
8. Bray F, Ferlay J, Soerjomataram I, Siegel RL, Torre LA, Jemal A. Global cancer statistics. GLOBOCAN estimates of incidence and mortality worldwide for 36 cancers in 185 countries. CA Cancer J Clin. 2018; 68(6): 394–424.
9. Caroline Lefeuvre, Hélène Le Guillou-Guillemette and Alexandra Ducancelle. A Pleiotropic Role of the Hepatitis B Virus Core Protein in Hepatocarcinogenesis, International Journal of Molecular Sciences. 2021)
10. Center MM, Jemal A. International trends in liver cancer incidence rates. Cancer Epidemiol Biomarkers Prev. 2011; 20(11): 2362–8.
11. P.R. Kiresee Saghana and S. Hemalatha.Potential of 4-Hydroxypropiophenone against Matrix Metalloproteinase 10: An In-silico docking study. Int. J. Adv. Res. Biol. Sci. 2016) 3(4): 8-12
12. Chen Shen, Xin Jiang, Mei Li and Yao Luo. Hepatitis Virus and Hepatocellular Carcinoma: Recent Advances, Cancers. 2023; 15: 533.
13. Cyriac A. Philips, Sasidharan Rajesh, Dinu C. Nair, Rizwan Ahamed, Jinsha K. Abduljaleel, Philip Augustine. Hepatocellular Carcinoma in 2021: An Exhaustive Update, Cureus 2021; 13(11): e19274.
14. Tanveer Hasan, Raza Murad Ghalib, Sayed Hasan Mehdi, P. K. Singh, S. S. R. Baqri. Normal Mode Analysis, Electronic Parameters and molecular docking study of 3, 5, 4'-Trihydroxy-6, 7-Dimethoxy-Flavone (Eupalitin) using First Principle. Asian J. Research Chem. 2017; 10(6): 789-797.
15. Mohmedyasin F. Mansuri, Shravan B. Rathod. Förster Resonance Energy Transfer Investigation between PPO and Coumarin 151 Dyes and Docking studies with Prolyl-tRNA Synthetase Conformers. Asian J. Research Chem. 2019; 12(6): 295-302.
16. Samir Zeroual, Ismail Daoud, Randa Gaouaoui, Said Ghalem. In vitro and Molecular Docking Studies of DPPH with Phoenix dactylifera L. (Deglet-Nour) Crude Fruits extracts and Evaluation of their Antioxidant Activity; Asian J. Research Chem. 2020; 13(1): 52-59.
17. Sindhu. T. J, Akhilesh K. J, Anju. Jose, Binsiya K. P, Blessy Thomas, Elizabeth Wilson. Antibacterial Screening of Clerodendrum infortunatum leaves: Experimental and Molecular docking studies.
18. Uzma Khan, Souvik Sur. Exploring DNA Binding of Benzothiazole-based Known Drugs: A Molecular Docking Investigation. Asian Journal of Research in Chemistry. 2023; 16(5): 383-8.
19. Sathish Kumar Mittapalli, J N Narendra Sharath Chandra, Jay

Prakash Soni, Ram Babu Tripathi, Iffath Rizwana. Virtual Screening and Pharmacophore Modeling for discovery of Biologically Active Natural Products as Inhibitors of Odorant-binding Proteins. Asian Journal of Research in Chemistry. 2024; 17(1): 17-4.

20. Amol Pawar, Chetan Salunke, Kailaspati Chittam, Anita B. Patil. Development of an Analytical Method of Glycyrrhizin by using High Pressure Liquid Chromatography. Res. J. Pharma. Dosage Forms and Tech.2020; 12(2): 49-52.
21. Sudhakar P, Poorana Pushkalai S, Sabarinath C, Priyadharshini S, Haripriya S . Molecular docking and synthesis of 1, 2, 4 - triazin analogue of diclofenac as potential ligand for parkinson's. Res. J. Pharmacology and Pharmacodynamics.2018; 10(1): 08-12.
22. Mohamed Zerein Fathima, T.S. Shanmugarajan, S. Satheesh Kumar, B.V.Venkata Nagarjuna Yadav. Comparative in Silico Docking Studies of Hinokitiol with Sorafenib and Nilotinib against Proto-Oncogene Tyrosine-Protein Kinase(ABL1) and Mitogen-activated Protein Kinase (MAPK) to Target Hepatocellular Carcinoma. Research J. Pharm. and Tech. 2017; 10(1): 257-262.
23. Jeyabaskar Suganya, Viswanathan T, Mahendran Radha, Nishandhini Marimuthu. In silico Molecular Docking studies to investigate interactions of natural Camptothecin molecule with diabetic enzymes. Research J. Pharm. and Tech. 2017; 10(9): 2917-2922.