Journal of Pharmaceutical Research International

Volume 35, Issue 22, Page 54-65, 2023; Article no.JPRI.103783
ISSN: 2456-9119
(Past name: British Journal of Pharmaceutical Research, Past ISSN: 2231-2919, NLM ID: 101631759)

In silico Molecular Docking Study of Some Novel Chalcone Derivatives as Anticancer Agents

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\Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

Article Information

DOI: 10.9734/JPRI/2023/v35i227416

Open Peer Review History:
This journal follows the Advanced Open Peer Review policy. Identity of the Reviewers, Editor(s) and additional Reviewers, peer review comments, different versions of the manuscript, comments of the editors, etc are available here: https://www.sdiarticle5.com/review-history/103783

Original Research Article

Received: 08/06/2023
Accepted: 11/08/2023
Published: 22/08/2023

ABSTRACT

We were encouraged to design and produce a new series of chalcone derivatives since there is a critical need for novel anticancer drugs with high selectivity for cancer cells. Chalcones are members of the flavonoid family that act as precursors in the production of flavonoids, which are plentiful in plants. Chalcones are significant starting points for synthetic modifications and serve as mediators in the synthesis of critical therapeutic compounds. Cancer is one of the leading causes of death globally. New compounds still need to be found to cure cancer. In certain cancer cells, chalcone and its derivatives have anticancer potential. Modern medication design frequently uses

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molecular docking to understand drug-receptor interaction. Docking studies are a crucial technique for enabling the organised use of the structural variety of natural products. The Molegro Virtual Docker 6.0 was used in this work to conduct docking investigations on natural anticancer drugs that contained chalcone. Using the software Molegro Virtual Docker 6.0, we docked the protein crystal structure of human T-cell leukaemia virus protease (2B7F) with several chalcone-based derivatives (AMP-1-56) for our study project. Among the compounds AMP-56, compounds AMP-40, 44, 45, 48, 49, 52, 55 and 56 exhibit good anticancer activity with human T-cell leukaemia virus protease (PDB-2B7F) as compared to the reference drug (Camptothecin). The results are still preliminary, and an experimental evaluation will soon be performed.

Keywords: Chalcone; cancer; therapeutic agents; molecular docking; anticancer.

1. INTRODUCTION

One of the most dangerous diseases of the 20th century, cancer is still prevalent in the 21st century and is continuing to spread. It is a class of illnesses marked by uncontrolled cell division that causes unusual tissue growth [1]. In the United States, there are anticipated to be 1,918,030 new cancer cases and 609,360 cancer deaths in 2022, with lung cancer being chalcone the primary cause of death accounting for around 350 of those fatalities daily [2].

According to research, 14,61,427 new cases of cancer are anticipated in India in 2022 (about 100.4 new cases of cancer are anticipated for every 100,000 people). One out of every nine Indians has a 90% lifetime risk of developing cancer. For both men and women, lung and breast malignancies were among the most prevalent types of cancer. Lymphoid leukaemia (boys: 29.2%; girls: 24.2%) accounted for the majority of children (0–14 years) malignancies. According to predictions, the number of cancer cases would rise by 12.8% between 2020 and 2025 [3].

The key factor and cause of the lack of effective anticancer medications are that cancer manifests in the human body through various pathways comprised of various cancer macromolecules, and it is very challenging for a single molecule or drug to inhibit all macromolecules simultaneously. B-cell lymphoma 2 (Bcl-2), vascular endothelial growth factor receptor 2 (VEGFR-2), cyclin-dependent protein kinase 6 (CDK-6), CDK-2, and IGF-1R kinase (insulin-like growth factor 1 receptor) are a few notable examples of cancer macromolecules [4].

Natural ingredients have historically and continuously been researched for potential new leads in pharmaceutical development. Research on plant-based antitumor agents will continue to yield new anticancer medications. An a, b-unsaturated enone is joined to two aromatic rings to form chalcones (1,3-diaryl-2-propen-1-ones), a subclass of the flavonoid family [5][6]. Many natural compounds, including curcumin, flavokawain, mill machine, and xanthohumol, depend on chalcones as their primary pharmacophores [7].

In the synthesis of flavonoids, which are found in a wide range of plants, chalcones, which are members of the flavonoid family, act as intermediates. Chalcones function as mediators in the production of useful pharmaceutical compounds that have a range of biological effects and are important building blocks for synthetic manipulations. The creation of chalcone derivatives and their significance in medicine have been the focus of several studies [8][9].

Chalcone derivatives may provide a good starting point for chemical-based organic chemical researchers to develop new compounds containing this moiety because of their similar or better activities compared to some of the requirements in a variety of biologically active compounds. Due to the adaptability of the chalcone family, broad-spectrum biological cancer applications can be created [10][11]. Numerous chalcone derivatives have demonstrated positive anti-inflammatory [12], anti-histaminic, anti-oxidant [13], anti-obesity, hypnotic activities [14], as well as antibacterial [15], antimalarial [16], anti-fungal [17], anti-leishmanial [18], anti-HIV, anti-diabetic [19] and anti-cancer activities [11].The anticancer potential of medicines or chemicals was evaluated using various in vitro, in vivo, and computational methodologies. Docking has been a popular technique among them for developing cancer medication candidates [20].

The use of computational biology and bioinformatics has the potential to alter how pharmaceuticals are created as well as speed up

the drug development process and cut expenses. Several techniques are used to find new compounds throughout the drug-developing process, which is facilitated and sped up by rational drug design (RDD) [21]. The drug molecule docking with the receptor (target) is one such technique. The receptor is the location of pharmacological action, which is ultimately in charge of the therapeutic impact (Richon,1994) [1]. The molecular modelling technique known as docking forecasts the preferred orientation of one molecule to another when they are linked together to create a stable complex. It is possible to forecast the degree of association or binding affinity between two molecules by knowing which orientation is favoured. To estimate the affinity and activity of the small molecule, docking is widely employed to determine the binding orientation of potential small molecule drugs to their protein targets [22].

2. MATERIAL AND METHODS

2.1 Materials Used

For the current work, we employed tools like Molegro Virtual Docker 6.0 (MVD), Molinspiration, and biological resources including PubChem, Drug Bank, and PDB (Protein Data Bank). Drug Bank is an innovative Bioinformatics/Cheminformatics tool that integrates thorough drug (i.e., chemical) data with thorough drug target (i.e., protein) data [26].

The PDB (Protein Data Bank) was created in Brookhaven National Laboratories (BNL) in 1971 and is the only global repository for structural data on biological macromolecules [27]. It includes macromolecule structural data obtained using X-ray crystallography, NMR, and other techniques. An independent research organisation called Molinspiration is dedicated to the creation and implementation of cutting-edge cheminformatics methods, particularly as they relate to the Internet. ChemDraw is a robust all-purpose chemical drawing and graphics software created by Labs to assist scientists in rapidly and simply designing molecules, processes, and schematic diagrams, computing chemical characteristics, and creating expert reports and presentations [28].

2.2 Preparation of Protein Structure

Bioinformatics is viewed as a developing discipline with the potential to greatly enhance how medications are discovered and introduced into clinical trials. Protein targets were downloaded from the database Protein Data Bank (PDB). 2B7F (Crystal structure of human T-cell leukaemia virus protease) is used for the docking process. Organism: Human T-cell leukaemia virus type I Sequence length of 2B7F is 116, this protein contains six chains i.e. chain A, chain B, chain D[auth C], chain E [auth D], chain G[auth E], and chain H [auth F] [29].

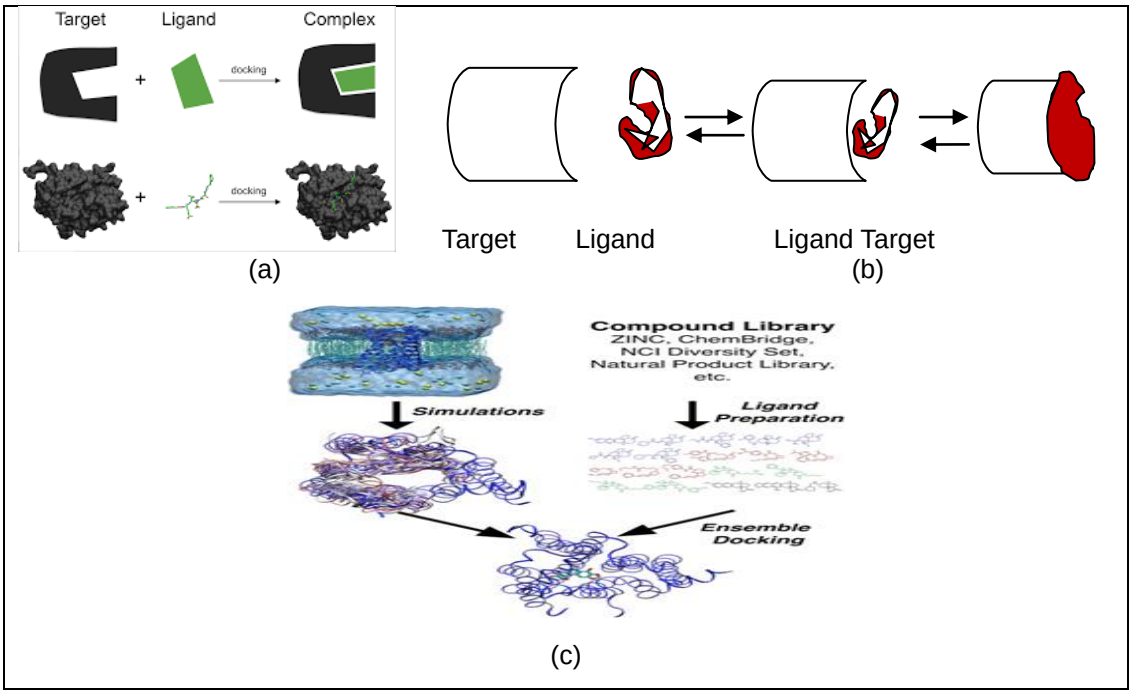

Fig. 1. Techniques of molecular docking: (a) Induced work docking[23]; (b) Lock and key docking[24]; and (c) Ensemble docking[25]

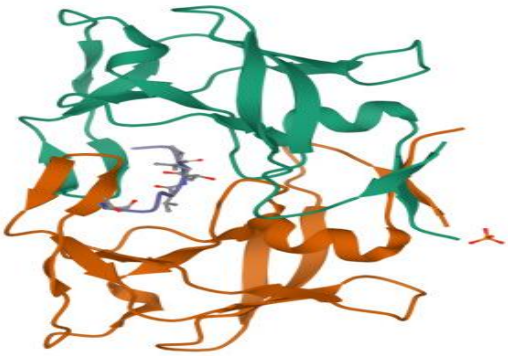

Fig. 2. Crystal structure of human T-cell leukaemia virus protease(2B7F)

2.3 Preparation of Ligand Structure

ChemDraw Professional 16.0 was used to sketch the structures of several chalcone derivatives, which was followed by Chem3D 16.0 to create the 3D structure. The MM2 technique [22] was used to optimise all the planned structures for energy reduction, and the Molegro Virtual Docker 6.0 interface turned the results into readable form. A protein 2B7F that was retrieved from the protein data library was used to find the powerful chalcone derivative. The Molegro Virtual Docker 6.0 was used for the docking investigation of chalcone derivatives with human T-cell leukaemia virus protease receptors.

2.4 Docking Simulations

The docking of chalcone derivatives with human T-cell leukaemia virus protease receptors was studied using the Molegro Virtual Docker 6.0 tool. The observations were analysed using Molegro Virtual Docker 6.0, which demonstrated close contact, hydrogen bonds, and hydrophilic and hydrophobic interactions. A scientist can use docking to digitally explore a library of compounds and predict the strongest binders using several score systems. It looks at how two molecules, such as pharmaceuticals and protease receptors for the human T-cell leukaemia virus, may fit together and dock. Drugs are compounds that attach to a receptor, inhibit its action, and thus serve as medications.

3. RESULTS AND DISCUSSION

For docking investigations, Molegro virtual docker 6.0 has been used. It displayed greater docking accuracy than other current docking software. MVD is effective in several recent experiments, as well as for economic and user-friendliness reasons.

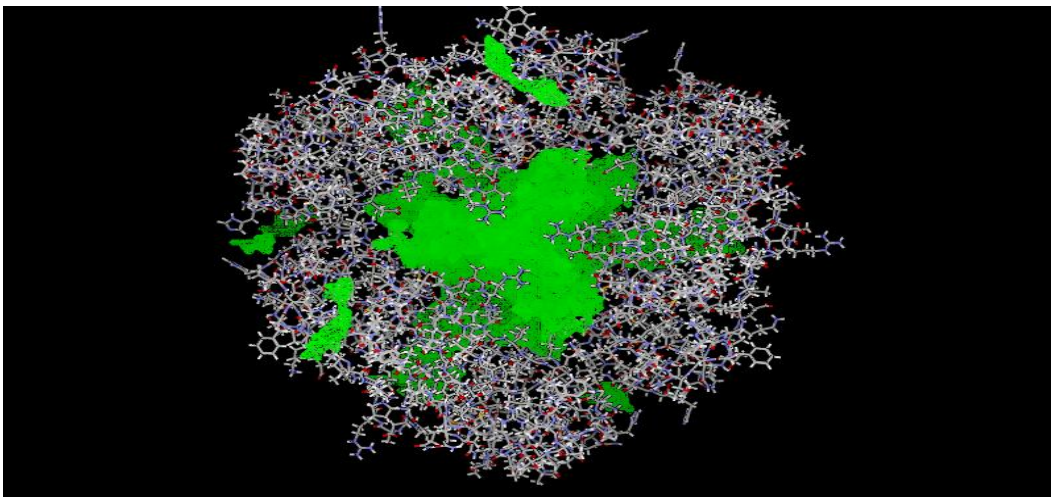

Fig. 3(a). The five cavities detected in molegro virtual docker in 2B7F

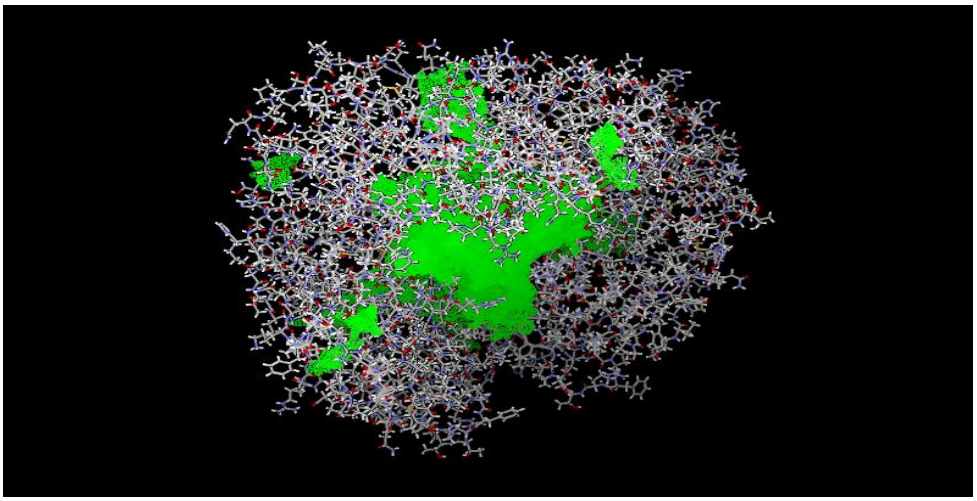

Fig. 3(b). The five cavities detected in molegro virtual docker in 2B7F

MVD's cavity identification system automatically finds potential binding sites (also known as cavities or active sites). In the example of the crystal structure of human T-cell leukaemia virus protease (PDB: 2B7F), the programme frequently identified cavities.

- Cavity [Vol= 6585.86]
- Cavity [Vol=98.816]
- Cavity [Vol=81.92]
- Cavity [Vol=60.416]
- Cavity [Vol=62.976]

3.1 Reference ligand (Camptothecin)

Moldock score, rerank score, docking score and H-bond of reference ligand were examined by docking method using Molegro virtual docker. The moldock score of the reference ligand was -75.9991. Rerank score of the reference ligand was observed as -63.225. The docking score of the reference structure was observed as -50.3042. The h-Bond of this reference ligand was -3.7369.

In comparison to the standard drug (Camptothecin), all hypothetical compounds showed good antitumor efficacy. Out of 56 compounds, eight have been shown to exhibit strong anticancer activity: AMP-40, AMP-44, AMP-45, AMP-48, AMP-49, AMP-52, AMP-55, and AMP-56. The docking results for 56 compounds are shown in Table 2.

3.2 Top 8 Chalcone Derivatives according to the Moldock Score

The best docking poses obtained based on the MVD moldock score, docking score, rerank score and hydrogen bond.

Reference ligand shows hydrogen bonding with protein at Gln107(C), and Gln108(C) after docking. It does not show any electrostatic interaction. Reference ligand shows steric interaction at Ser89(C), Pro7(D).

3.3 The Docking Poses for All These Eight Derivatives are

The interaction of derivatives with protein 2B7F was shown: First derivative having MVD name Unknown1_40 shows hydrogen bonding at Gln107(C), Asp36(C). It shows no electrostatic interaction. It shows steric interaction at Gln108(C), Gln107(C), Asp104(C), Pro7(D).

The second derivative (44^{th} derivative) having MVD name Unknown1_44 shows hydrogen bonding at Arg9(F). It shows no electrostatic interaction. It shows steric interaction at Val12(F), Ala8(F), Arg10(F), Pro7(F), Asp36(E), Met37(E).

The third derivative (45^{th} derivative) having MVD name Unknown1_45 shows hydrogen bonding at Arg10(F), Asp36(E). It shows no electrostatic interaction. It shows steric interaction at Arg10(F), Ala8(F), Asp36(E).

The fourth derivative (48^{th} derivative) having MVD name Unknown1_48 shows hydrogen bonding at Pro7(D), Arg9(D), Asp6(D). It shows no electrostatic interaction. It shows steric interaction at Arg9(D), Arg10(D), Asp36(C), Pro7(D), Asp6(D).

Table 1. Docking observation of 56 chalcone derivatives

Sr. No.	M.V.D. name	MolDock Score	Rerank Score	H-bond	Docking Score
	Reference Drug	**-75.9991**	**-63.225**	**-3.7369**	**-50.3042**
1	Unknown1	-70.9151	-56.114	0	-68.5816
2	Unknown1_1	-66.7386	-52.6321	-1.10439	-64.9592
3	Unknown1_2	-70.6852	-54.9392	0	-61.1169
4	Unknown1_3	-68.6865	-48.9362	-2.27086	-57.8369
5	Unknown1_4	-61.613	-51.0934	-3.9948	-59.1487
6	Unknown1_5	-67.8585	-53.5611	-2.77259	-64.4364
7	Unknown1_6	-66.5594	-52.5179	0	-65.7576
8	Unknown1_7	-69.3261	-53.5997	-1.64112	-67.7813
9	Unknown1_8	-63.3384	-32.7058	-1.12383	-61.9383
10	Unknown1_9	-67.3191	-51.6946	0	-57.4056
11	Unknown1_10	-65.1678	-50.885	0	-63.7428
12	Unknown1_11	-65.5431	-51.3613	0	-56.12
13	Unknown1_12	-63.7637	-49.9888	0	-62.8938
14	Unknown1_13	-67.6455	-54.069	-0.129882	-69.5306
15	Unknown1_14	-74.1066	-60.8597	-5	-55.9882
16	Unknown1_15	-66.0369	-52.4835	-1.60196	-65.4791
17	Unknown1_16	-76.3223	-60.3786	-1.04354	-73.7271
18	Unknown1_17	-74.9651	-47.0231	-0.0378454	-66.9754
19	Unknown1_18	-73.023	-58.0601	-1.845	-68.9731
20	Unknown1_19	-67.676	-52.6332	-2.23919	-62.7867
21	Unknown1_20	-64.1079	-50.8493	-0.0382037	-64.9173
22	Unknown1_21	-60.931	-47.9713	-0.236345	-61.1359
23	Unknown1_22	-65.1667	-51.5752	-0.0504573	-66.0923
24	Unknown1_23	-68.0299	-48.7877	-2.6896	-64.4066
25	Unknown1_24	-71.9791	-43.9372	-0.460705	-71.3025
26	Unknown1_25	-73.3614	-59.6856	-3.02394	-57.2556
27	Unknown1_26	-68.4003	-50.9526	-2.5	-59.4652
28	Unknown1_27	-67.3828	-53.7432	-3.33953	-68.101
29	Unknown1_28	-64.9085	-39.4629	-1.91212	-64.7513
30	Unknown1_29	-62.2344	-55.4742	-2.4364	-59.8501
31	Unknown1_30	-67.6695	-52.4527	-1.03451	-67.4183
32	Unknown1_31	-67.5743	-53.4461	-1.74037	-67.0116
33	Unknown1_32	-72.9389	-56.7529	-1.93871	-68.4101
34	Unknown1_33	-69.5689	-55.2064	0	-67.43
35	Unknown1_34	-69.8514	-14.1339	-1.2314	-67.0261
36	Unknown1_35	-71.1251	-54.7935	-1.55812	-72.1664
37	Unknown1_36	-71.5621	-45.7397	-4.01854	-63.1455
38	Unknown1_37	-72.0834	-56.8656	-2.07337	-64.3349
39	Unknown1_38	-69.5656	-50.568	0	-68.0192
40	Unknown1_39	-72.3618	-58.7482	-1.46078	-65.1347
41	Unknown1_40	-82.249	-53.6024	-8.40025	-80.2312
42	Unknown1_41	-69.4549	-56.5282	-1.13262	-67.2436
43	Unknown1_42	-65.9078	-39.438	-6.95591	-57.605
44	Unknown1_43	-90.1974	-64.8504	0	-80.0839
45	Unknown1_44	-86.9148	-69.0287	-1.86115	-80.2322
46	Unknown1_45	-85.1072	-67.9218	-2.93547	-82.5954
47	Unknown1_46	-77.8863	-62.3982	0	-72.8396
48	Unknown1_47	-68.6175	-55.3666	-1.26295	-69.4548
49	Unknown1_48	-75.3738	-55.8692	-7.50431	-73.5146
50	Unknown1_49	-76.6345	-59.3305	-8.2543	-75.4349
51	Unknown1_50	-70.7739	-54.5791	-3.16321	-69.2101
52	Unknown1_51	-89.7539	-71.9074	-1.48893	-80.1209

Sr. No.	M.V.D. name	MolDock Score	Rerank Score	H-bond	Docking Score
	Reference Drug	**-75.9991**	**-63.225**	**-3.7369**	**-50.3042**
53	Unknown1_52	-91.3642	-72.4414	-1.93425	-86.3559
54	Unknown1_53	-75.4889	-53.7355	0	-72.2653
55	Unknown1_54	-77.5313	-51.1217	-2.9036	-69.7982
56	Unknown1_55	-93.4426	-75.0979	-1.85205	-86.1485
57	Unknown1_56	-85.8879	-67.4836	-1.81418	-80.6948

Table 2. Docking observation for top eight derivatives

Derivative	M.V.D. name	Moldock score	Rerank score	H bond	Docking score
40	Unknown1_40	-82.249	-53.6024	-8.40025	-80.2312
44	Unknown1_44	-86.9148	-69.0287	-1.86115	-80.2322
45	Unknown1_45	-85.1072	-67.9218	-2.93547	-82.5954
48	Unknown1_48	-75.3738	-55.8692	-7.50431	-73.5146
49	Unknown1_49	-76.6345	-59.3305	-8.2543	-75.4349
52	Unknown1_52	-91.3642	-72.4414	-1.93425	-86.3559
55	Unknown1_55	-93.4426	-75.0979	-1.85205	-86.1485
56	Unknown1_56	-85.8879	-67.4836	-1.81418	-80.6948

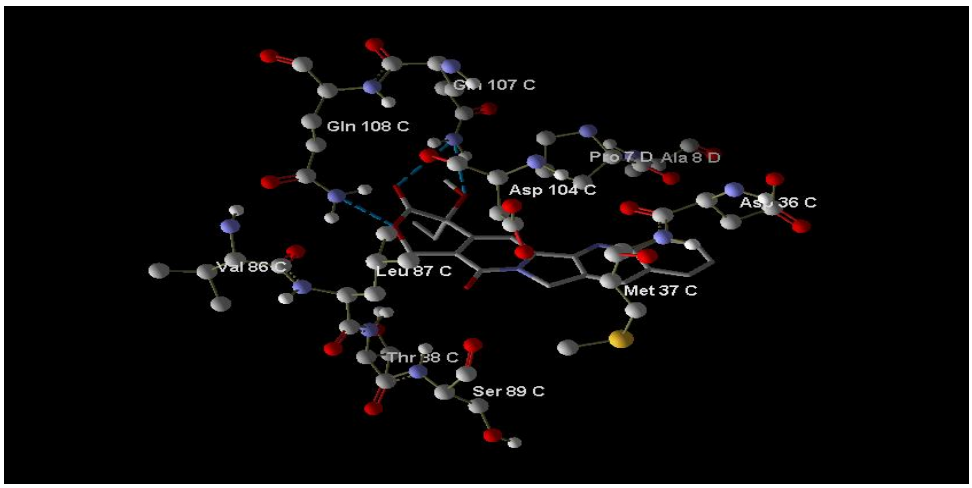

Fig. 4. Docking image of camptothecin reference structure in MVD

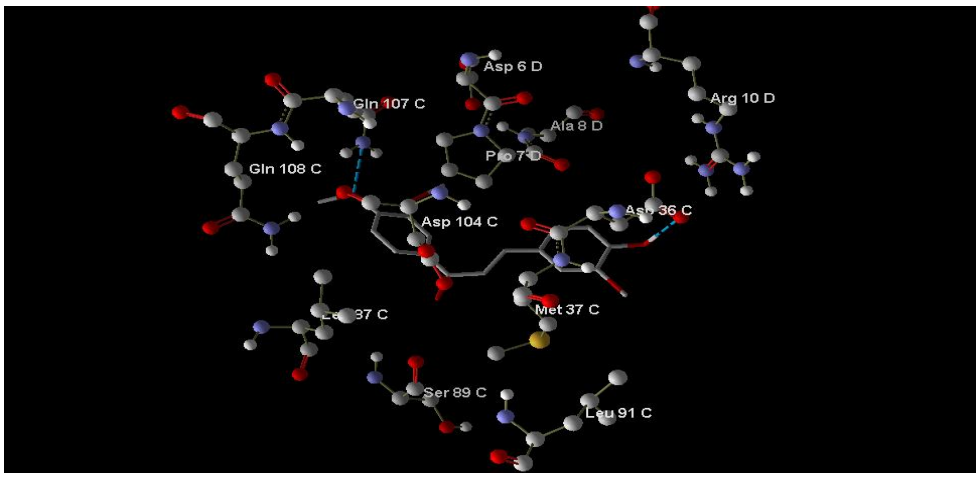

Fig. 5. Docking pose of derivative 40

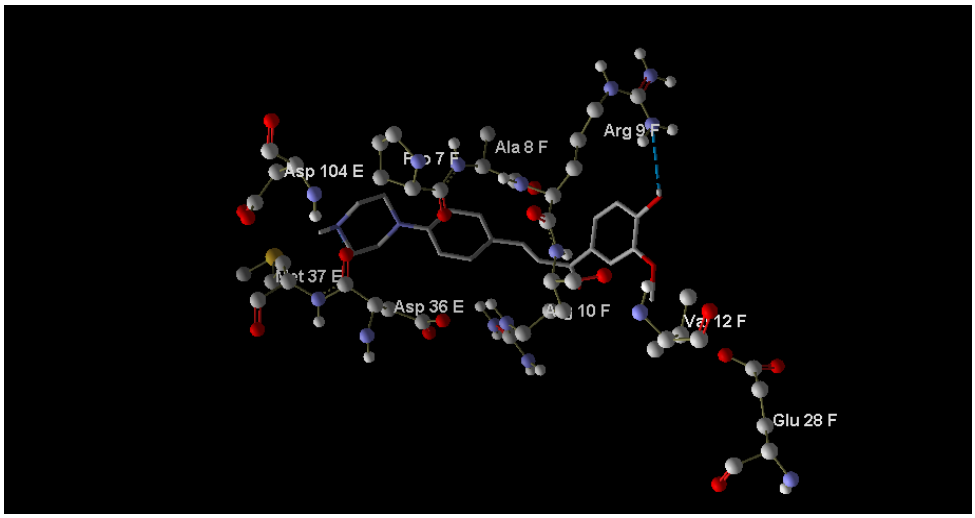

Fig. 6. Docking pose of derivative 44

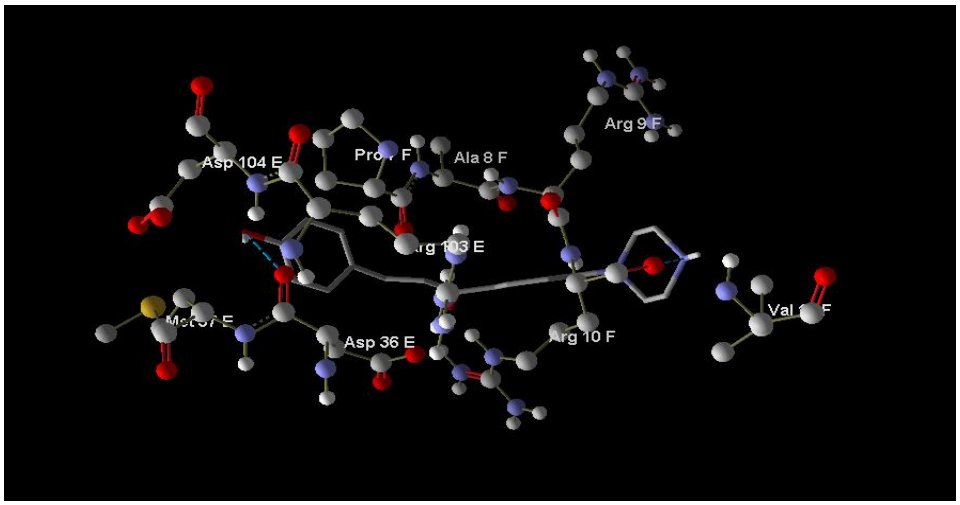

Fig. 7. Docking pose of derivative 45

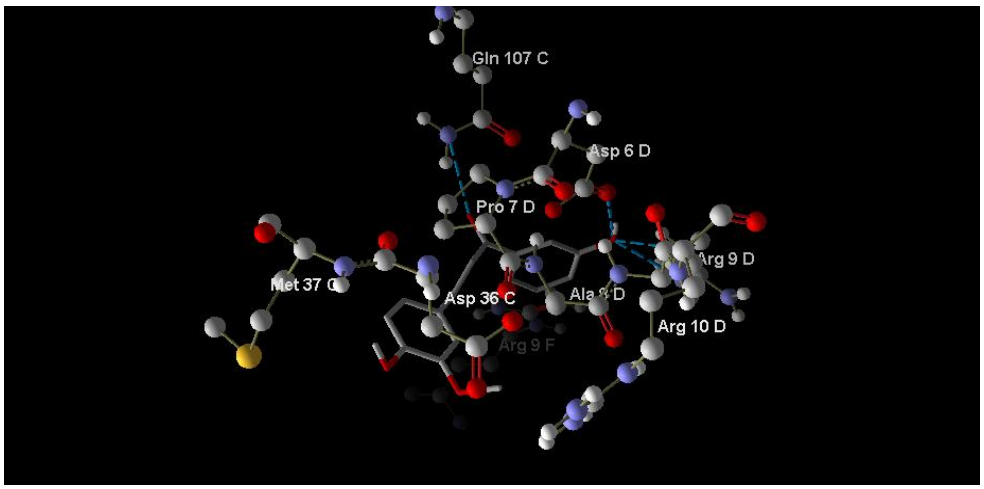

Fig. 8. Docking pose of derivative 48

The fifth derivative (49th derivative) having MVD name Unknown1_49 shows hydrogen bonding at Pro4(F), Arg103(E). It shows no electrostatic interaction. It shows steric interaction at Leu5(F), Asp6(F), Pro4(F), Arg103(E).

The sixth derivative (52nd derivative) having MVD name Unknown1_52 shows hydrogen bonding at Arg9(F). It shows no electrostatic interaction. It shows steric interaction at Ala8(F), Arg10(F), Pro7(F).

The seventh derivative (55th derivative) having MVD name Unknown1_55 shows hydrogen bonding at Arg9(F). It shows no electrostatic interaction. It shows steric interaction at Ala8(F), Arg10(F), Pro7(F), Asp104(E).

The eighth derivative (56th derivative) having MVD name Unknown1_56 shows hydrogen bonding at Arg9(F). It shows no electrostatic interaction. It shows steric interaction at Ala8(F), Pro7(F), Asp36(E).

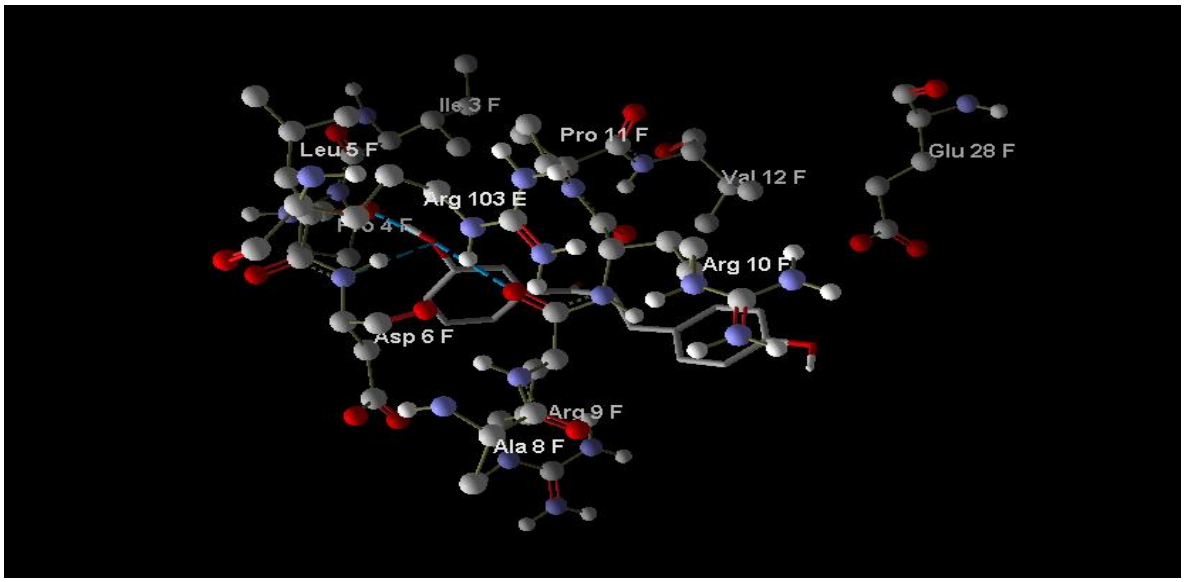

Fig. 9. Docking pose of derivative 49

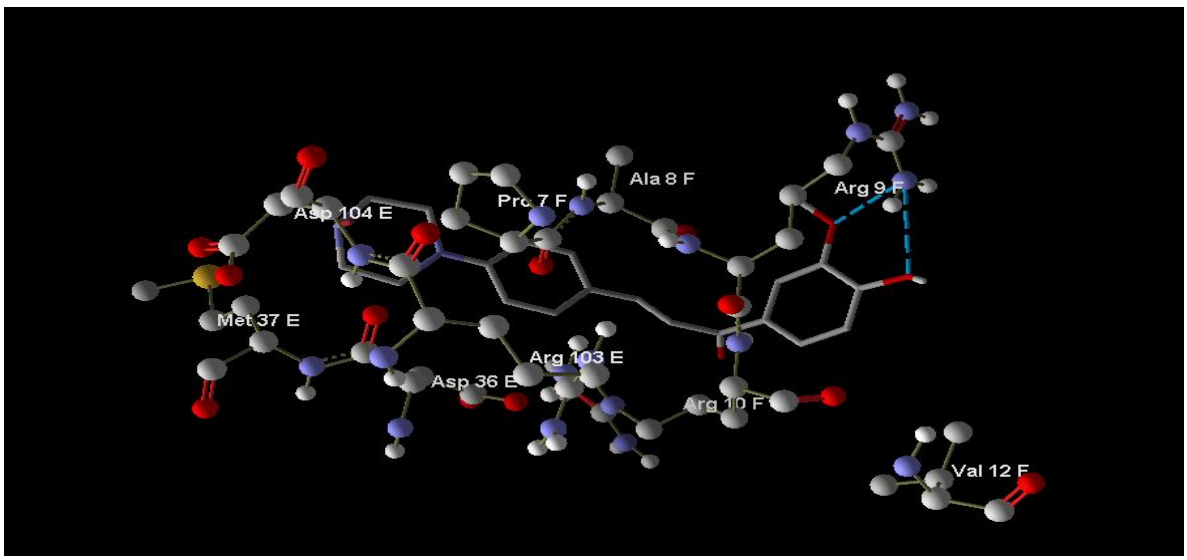

Fig. 10. Docking pose of derivative 52

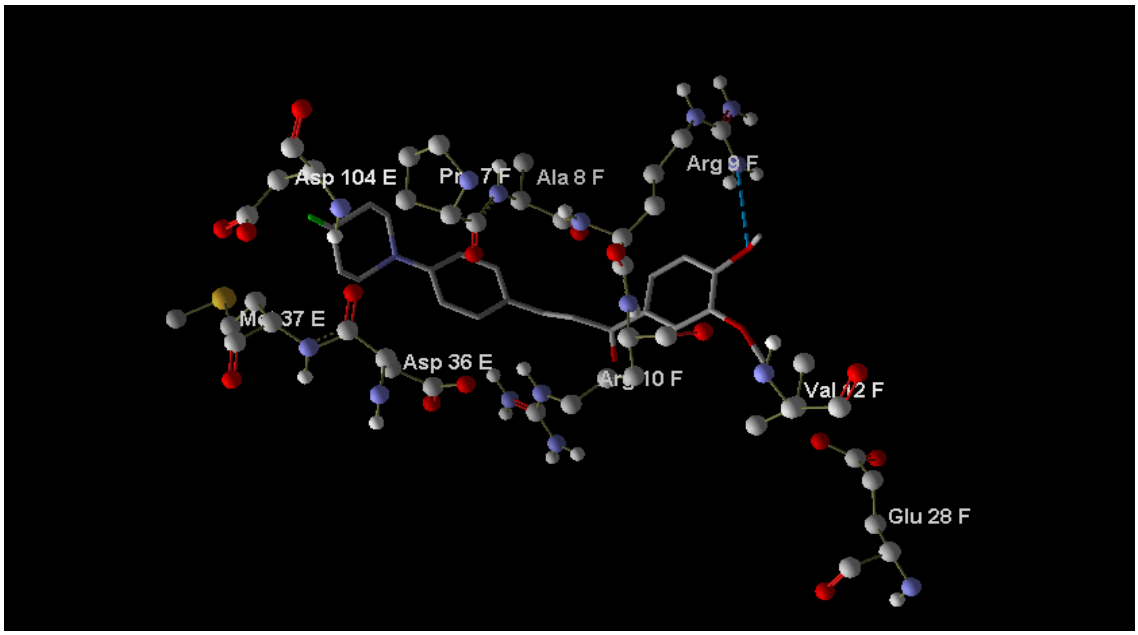

Fig. 11. Docking pose of derivative 55

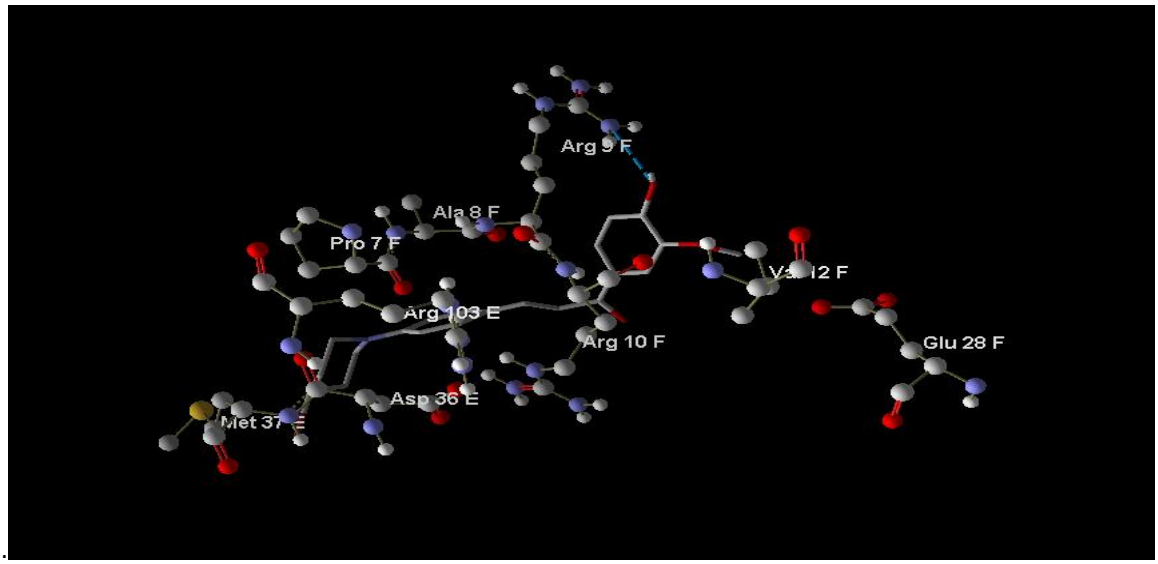

Fig. 12. Docking pose of derivative 56

4. CONCLUSION

The MVD was effectively used to carry out molecular docking investigations between the human T-cell leukaemia virus protease (PDB: 2B7F) and several anticancer drugs. To increase the potency of the original molecule, new analogues were created from the compound that had the best docking score for the protein target. Molecular docking was used in this work to investigate the binding mechanism and to connect the activity of chalcone derivatives with the docking score. The results of this study might be applied to the research and development of new compounds with enhanced anti-cancer action. When compared to the reference drug (Camptothecin), compounds AMP-40,44,45,48,49,52,55 and 56 exhibit the best-fit findings, according to the docking result.

ACKNOWLEDGEMENT

Authors are highly thankful to Abhilashi University for providing the necessary facilities.

CONSENT AND ETHICAL APPROVAL

It is not applicable.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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Peer-review history:
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