



RESEARCH ARTICLE

Structure-based computational analysis of jamun (*Syzygium cumini*) seed phytochemicals targeting the type 2 diabetes-associated human dipeptidyl peptidase 4 (DPP4) protein

Sanjoy Majumder^{1,2*} & Gagan Kumar Panigrahi^{3*}

¹School of Biotechnology, Centurion University of Technology and Management, Bhubaneswar 752 050, Odisha, India

²Jagannath Majumder Research Foundation (JMRF), Santir Bazar 799 144, Tripura, India

³School of Applied Sciences, Centurion University of Technology and Management, Bhubaneswar 752 050, Odisha, India

*Email: majumdersbt@gmail.com; gagan.panigrahi@cutm.ac.in

OPEN ACCESS

ARTICLE HISTORY

Received: 31 July 2025

Accepted: 05 November 2025

Available online

Version 1.0 : 01 January 2026

Additional information

Peer review: Publisher thanks Sectional Editor and the other anonymous reviewers for their contribution to the peer review of this work.

Reprints & permissions information is available at https://horizonpublishing.com/journals/index.php/TCB/open_access_policy

Publisher's Note: The article processing was done by atom e-Publishing, Thiruvananthapuram, India. Horizon e-Publishing Group remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Copyright: © The Author(s). This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution and reproduction in any medium, provided the original author and source are credited (<https://creativecommons.org/licenses/by/4.0/>)

CITE THIS ARTICLE

Sanjoy M, Gagan KP. Structure-based computational analysis of jamun (*Syzygium cumini*) seed phytochemicals targeting the type 2 diabetes-associated human dipeptidyl peptidase 4 (DPP4) protein. Trends in Current Biology. 2025; 4(1): 20-26. <https://doi.org/10.14719/tcb.9437>

Abstract

Type 2 Diabetes Mellitus (T2DM) is a metabolic chronic illness that imposes a health challenge, worldwide. Although there are conventional antidiabetic drugs available, there are still increasing demands of safer and cheaper drugs. *Syzygium cumini* (jamun) is a traditional medicinal plant that contains numerous bioactive phytochemicals that can be utilised towards diabetes control in terms of therapeutic potential. *In silico* drug discovery method was adopted in this work to screen some of the phytochemicals in *S. cumini* seeds against the target protein dipeptidyl peptidase 4 (DPP4), which is suspected to regulate glucose metabolism. The binding affinities and interaction patterns were determined by molecular docking and the ADMET (Absorption, Distribution, Metabolism, Excretion and Toxicity) of compounds was analyzed to determine pharmacokinetics and safety profile of the compounds. The binding affinities of three compounds quercetin, ellagic acid and β -sitosterol were found in a good range and the ADMET profile of these compounds was suggesting that these compounds may be used as potential hits to anti-diabetic drug discovery. *In vitro* and *in vivo* studies are needed to confirm these findings further.

Keywords

diabetes mellitus; DPP4; jamun; molecular docking; phytochemicals

Introduction

T2DM is a long-term metabolic disease that is manifested through insulin resistance, poor insulin response and raised levels of glucose in the blood. With the prevalence of T2DM across the globe continuing to spiral upwards, T2DM is becoming a heavy load on the healthcare system in the population and it predisposes people to the more serious diseases including cardiovascular disease, neuropathy, nephropathy and retinopathy (1-3). Although several antidiabetic medications can be used, they are associated with several limitations that include the presence of undesirable side effects, unaffordable pricing and diminished efficacy with time, a fact that highlights that safer and affordable and efficacious alleviating agent should be sought out.

DPP4 is the enzyme that breaks down incretin hormones including glucagon-like peptide-1 (GLP-1) and gastric inhibitory peptide (GIP) this enzyme has become one of the promising therapeutic targets in treatment of T2DM (4-6). DPP4 inhibitors restore the effects of the incretin, increases insulin release and improve blood sugar levels (7). Several synthetic DPP4 inhibitors are in clinical practice, but there is still a safety concern. This has spurred an increased interest in the investigation of natural products especially the phytomolecule based products in respect of their potential antidiabetic effects and reduced toxicity.

Syzygium cumini or jamun (also called Indian blackberry) is a wild type of fruit plant that has been employed commonly in systems of traditional medicine in treating diabetes mellitus. Its seeds, leaves, bark and fruits consist of diverse kinds of bioactive phytochemicals (8-10). The seeds of jamun are a great source of bioactive phytochemicals which have great therapeutic implications. The seeds are rich in a wide range of phenolic compounds, flavonoids, tannins, terpenoids, saponins and glycosides as well as alkaloids which make them great antioxidants, anti-diabetic and anti-inflammatory agents (11-13). Key bioactive compounds identified in jamun seeds are jambosine, ellagic acid, gallic acid, quercetin, catechin, myricetin, β -sitosterol and corilagin as well as, essential fatty acids and micronutrients (14). It is because of this broad phytochemical profile that jamun seeds have been traditionally employed in ayurvedic medicine, in the treatment of diabetes mellitus, digestive disorders and issues of the cardiovascular system, factors that make them a good potential source of plant-derived therapeutic agents (15,16). The understanding of ethnomedicines or traditional medicines has been transmitted across generations, laying the groundwork for ongoing research into drug discovery from natural sources (17-19). Many studies, including *in vitro* experiments, animal model studies and clinical trials, have shown that phytochemicals have anti-inflammatory, anti-bacterial, antiviral and free radical scavenging properties (20,21). Numerous phytochemicals have the potential to interact with multiple proteins involved in glucose metabolism, including AMPK, GLUT4, α -glucosidase, aldose reductase and PPAR γ . Such multi-target effects could enhance insulin sensitivity, glucose uptake and metabolic regulation, suggesting a broader antidiabetic potential (22-25). These multi-target interactions may contribute to their overall antidiabetic potential by modulating insulin signalling, enhancing glucose uptake and reducing postprandial hyperglycemia. Such pleiotropic effects suggest that these phytochemicals could act synergistically, supporting their effectiveness against T2DM. Experimental studies are required to confirm these interactions and their functional relevance in T2DM. In

most cases phytochemicals are considered to be less toxic than the conventional therapies and can be an option for treating numerous diseases, with or without conventional drugs.

This research is carried out by using an *in silico* process to screen and assess phytochemicals present in the jamun tree against the DPP4 protein. The binding affinity, the stability and the drug-like properties to predict the pharmacokinetics of the selected compounds can be determined using computational techniques like molecular docking and ADMET analysis (26). The goal of this computational screening is to facilitate discovery of potential lead compounds that would be evaluated in the *in vitro* and *in vivo* platform in the development of plant-based medicines used to treat T2DM. Although *in silico* tests like molecular docking and ADME prediction offer good preliminary information about the possible efficacy and pharmacokinetic behaviour of potential phytochemicals, they also have some critical disadvantages. They are unable to model the entire complexity of biological systems such as metabolism, off-target effects and pharmacodynamics. As such, to ensure the antidiabetic potential, safety and therapeutic importance of these compounds, experimental validation (*in vitro* and *in vivo* study) is required.

Materials and Methods

A flowchart diagram of this current study of screening of phytochemicals present in jamun seeds against human DPP4 protein is presented in Fig. 1.

Selection and preparation of ligands

For selecting the phytochemicals, we have reviewed previously published literatures demonstrating the antidiabetic potential of the extracts of jamun fruits and seeds (27,28). Based on literature survey we have selected bioactive phytochemicals presents in jamun seeds and prepared a ligand library. Chemical structures of these phytochemicals were obtained from the PubChem database in SDF format. To identify potential inhibitors of DPP4 protein, molecular

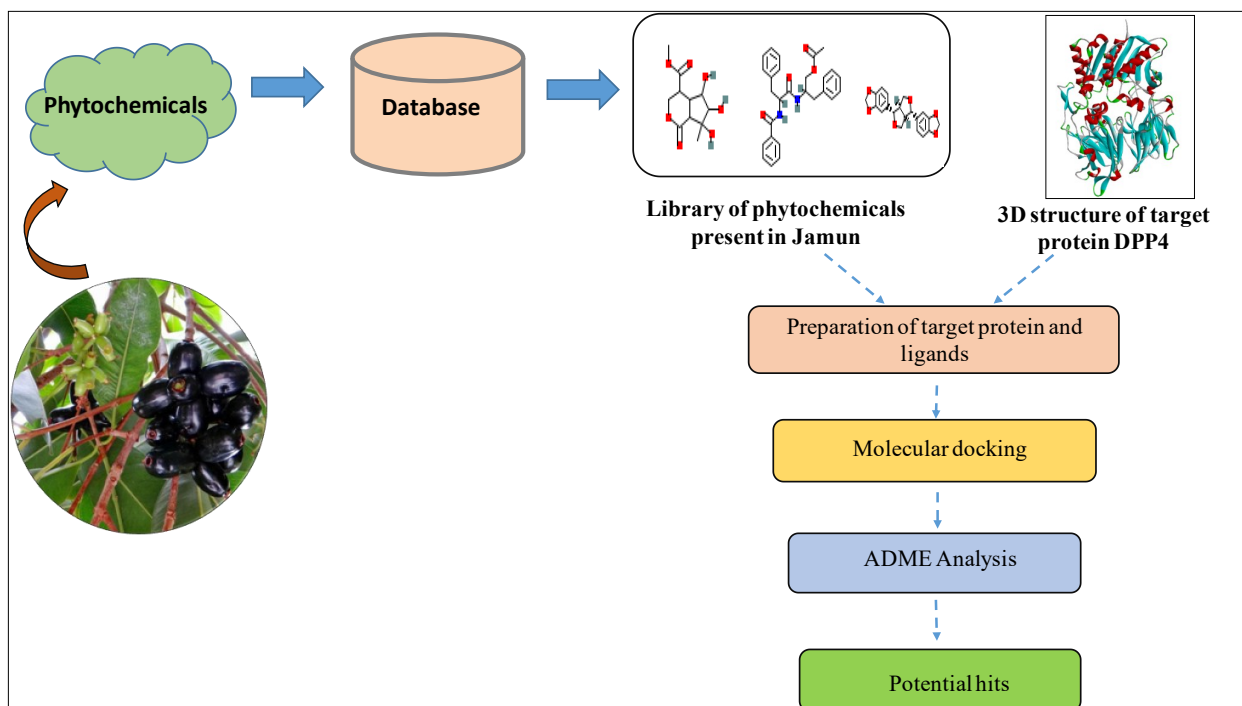


Fig. 1. Representing flow chart of the study of identifying the potential inhibitors of human DPP4 protein using molecular docking approach and *in silico* ADME analysis.

docking of this ligand library is to be done against the DPP4 protein. Before proceeding further to molecular docking step, energy minimization and optimization of these phytochemicals were done using OpenBabel (29) in linux environment. Then these compounds were converted and saved in pdbqt format.

Preparation of receptor protein (DPP4)

The three-dimensional (3D) structure of the of human DPP4 protein was downloaded from the RCSB Protein Data Bank (PDB ID: 3W2T) for docking purpose. Prior to molecular docking we have processed the 3D structure of this protein using AutoDockTools 1.5.7. (30). In this preprocessing step removal of water molecule and other hetero atoms were done, added polar hydrogens and Kollman charges. Then generated a grid box covering all the binding pockets present in the target protein.

Molecular docking based screening of potential inhibitor of DPP4

For this molecular docking study, we have used AutoDock Vina version 1.2.5. (31). The grid box was defined around the DPP4 with dimensions of 126 Å x 126 Å x 126 Å and a spacing of 0.375Å. Grid center was fixed as 48.64(X); 60.1(Y); 31.941(Z). Exhaustiveness was set to 8 and 10 binding modes were generated for each ligand. These parameters were chosen for DPP4 to ensure reliable binding predictions. This approach ensures that the docking procedure captures all relevant ligand conformations and binding poses, providing a strong basis for evaluating potential interactions. To screen for potential inhibitors of human DPP4, performed a blind docking of our prepared ligand library against the target DPP4 protein.

Drug-likeness and ADME profiling

Pharmacokinetic properties (ADME) are another crucial part of drug discovery process because they help in estimating absorption, distribution, metabolism and excretion of a compound in the body. ADME profiling gives important clues on the drug-likeness, bioavailability and the overall suitability of molecules to be developed further. In this study, pharmacokinetic profiles of the phytochemicals were predicted using computational tools. Phytochemicals screened through molecular docking study has undergone *in silico* ADME analysis using Swiss ADME server (32). In this analysis we have checked for any violations of Lipinski's rule along with other significant parameters (33).

Results and Discussion

Molecular docking

In computational drug designing molecular docking is a widely used method that helps to identify potential drug candidates against various disease targets. This advanced computational method can save a significant amount of energy, time and costs in the drug discovery process by screening large libraries of potential drug compounds in a very short span of time. In our study, we have screened phytochemicals of jamun seeds against human DPP4 using Autodock Vina 1.2.5. In this current study, for selecting the compounds we have considered a binding energy threshold of -8.0 kcal/mol, which was decided based on previous docking studies reporting that FDA-approved DPP4 inhibitors exhibit binding energies around this value (34,35). Based on the binding energy score, we have shortlisted top three bioactive phytocompounds (binding energy score less than -8.0 kcal/mol). These compounds are namely quercetin, ellagic acid and β -sitosterol which are found to have a lower binding energy of -8.315, -8.18 and -8.111 kcal/mol, respectively (Table 1). Docking results of these compounds also shows their higher binding affinity towards DPP4 in comparison to previously reported binding energy score of a significant DPP4 inhibitor sitagliptin, which is around -7.7 kcal/mol, indicating potential efficacy of these phytochemicals in modulating the function of DPP4 protein (34,35). The binding affinity and details of various molecular interactions of these three molecules with human DPP4 are displayed in Table 1.

Evaluation of drug likeness

The identified phytochemicals quercetin, ellagic acid and β -sitosterol demonstrate strong biological relevance due to their reported antidiabetic, antioxidant and anti-inflammatory properties. Additionally, ADME analysis reveal favorable pharmacokinetic profiles, suggesting that these natural phytochemicals could serve as safe and effective lead candidates for further development as DPP4 inhibitors. Each of the three phytochemicals met most of the criteria of Lipinski's rule of five, which is representative of drug-likeness of a compound. Quercetin and ellagic acid passes all the criteria of this rule, however β -sitosterol was highly lipophilic. β -sitosterol has one Lipinski violation as it has high LogP value, greater than the recommended value of 5, indicating its high lipophilicity which may constrain oral bioavailability and solubility. However, with its favourable membrane permeability, stable metabolism, along with excellent DPP4 binding affinity, it has the potential to be an excellent lead structure. To alleviate the solubility constraints, favourable

Table 1. Results of molecular docking showing binding energy scores and various molecular interactions between RNP domain of human DPP4 and selected phytochemicals present in jamun

Sl.No	Phytochemical	Binding energy (kcal/mol)	Residues of DPP4 protein involved in different types of molecular interactions
1	Quercetin	-8.315	Hydrogen bond: ARG125; SER 630; TYR 662; ASN710 Pi-pi stacked: PHE 357 Pi-Anion: GLU206 Van der Waals Interactions: GLU205, SER209; TYR547; VAL711; HIS740
2	Ellagic Acid	-8.18	Hydrogen bond: ASN92; PHE95; ILE102 Van der Waals Interactions: ILE76; LEU90; GLU91; SER93; THR94; SER101; ASN103; ASP104; TYR105 Hydrogen bond: TYR662 Pi-sigma: PHE357
3	β -Sitosterol	-8.111	Pi-Alkyl: ILE405; TYR666 Van der Waals Interactions: ARG125; GLU205; GLU206; SER209; ARG356; ARG358; TYR547; TYR585; SER630; ASN710

formulation strategies can be adopted in order to optimize its drug-like characteristics. Overall analysis of the drug-likeness indicates that, these phytochemicals from jamun seeds shows positive pharmacokinetic properties which makes them potential hits. The results of the *in silico* ADME analysis of the top three phytochemicals using Swiss ADME server are shown in Table 2.

Several phytochemicals possess the anti-diabetic properties. This docking outcome indicates that many phytochemicals might interact with amino acid residues of human DPP4 protein effectively. In the present study, we explored the potential of phytochemicals present in Jamun seeds against the human DPP4 and based on the molecular docking results and *in silico* analysis of ADME properties three phytochemicals were selected, namely quercetin, ellagic acid and β -sitosterol for further evaluation. In this study we have used Biovia Discovery Studio Visualizer to generate 2D and 3D plots of molecular interactions between protein and ligands. The 3D plot mainly shows the different bonded interactions. To show the various bonded as well as non-bonded (eg. Van der Waals) molecular interactions between DPP4 and phytochemicals we have generated 2D plot. Here we have shown both 3D and 2D plots of molecular interactions between protein and the selected ligands with high binding affinity (Fig. 2-4).

Conclusion

This study used the *in silico* methods to investigate the pharmacological effect of jamun (*Syzygium cumini*) seeds against the DPP4 protein, which is major target that contributes to the causation of T2DM. Medicinal plants such as jamun are important in terms of drug discovery as they are known to be a source of bioactive compounds, which can be used in the management of diabetes, as identified through the study. Three phytochemicals present in the jamun seeds represented a high binding affinity and stable interaction at the active site of the DPP4 protein. These phytochemicals shown good binding energy in molecular docking hence portray their ability as potential modulators of the activity of the DPP4 protein. Further this result establishes a basis to carry out future *in vitro* and *in vivo* studies as well as Structure-Activity Relationships (SAR) for further substantiating the antidiabetic potential, pharmacokinetics and safety standards of the identified phytochemicals. Besides DPP4, the screened phytochemicals can also interact with other various proteins related to glucose metabolism such as AMPK, GLUT4, α -glucosidase, aldose reductase, PPAR γ among others. These multi-target effects have the potential to increase insulin sensitivity, glucose uptake and metabolic regulation and indicate a more extensive antidiabetic potential.

Table 2. ADME properties of the three selected phytochemicals

Sl. No.	Phytomolecule	MW	Rotatable bond	H-bond acceptor	H-bond donor	TPSA	BBB permeant	Lipinski violation	Bioavailability Score
1.	Quercetin	302.24	1	7	5	131.36	No	No	0.55
2.	Ellagic Acid	302.19	0	8	4	141.34	No	No	0.55
3.	Beta-Sitosterol	414.71	6	1	1	20.23	No	Yes(1)	0.55

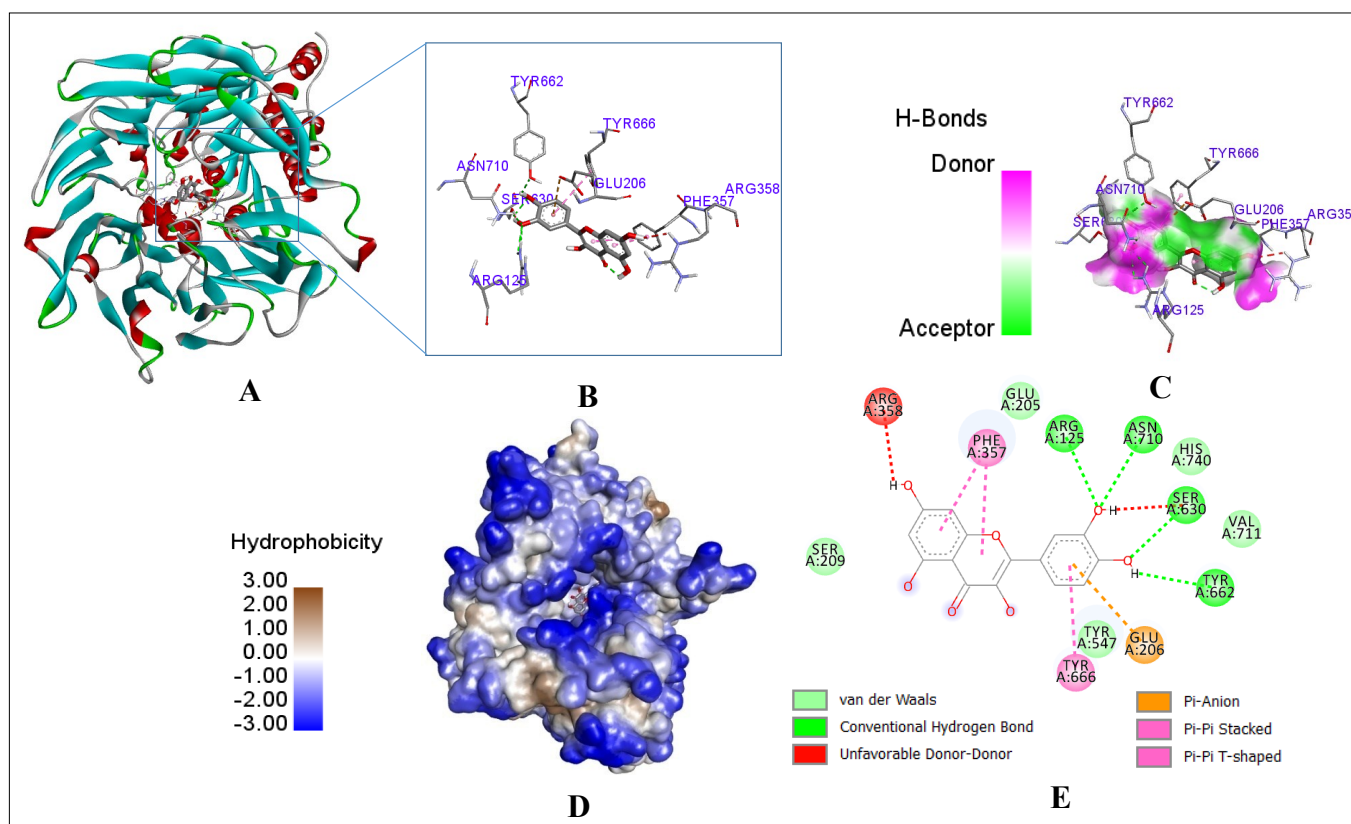


Fig. 2. 2D and 3D interaction diagram of quercetin with the active site residues of the human DPP4 protein (PDB ID:3W2T).

(A) Complex of DPP4 and quercetin; (B) Close view of pocket with quercetin; (C) Hydrogen bond donor and acceptor surface representation of the complex; (D) Hydrophobicity surface representation of the human DPP4 in complex with quercetin; (E) 2D representation of different types of interactions with quercetin

This compound forms hydrogen bonds with key residues ARG125, ASN710, SER630 and TYR 662

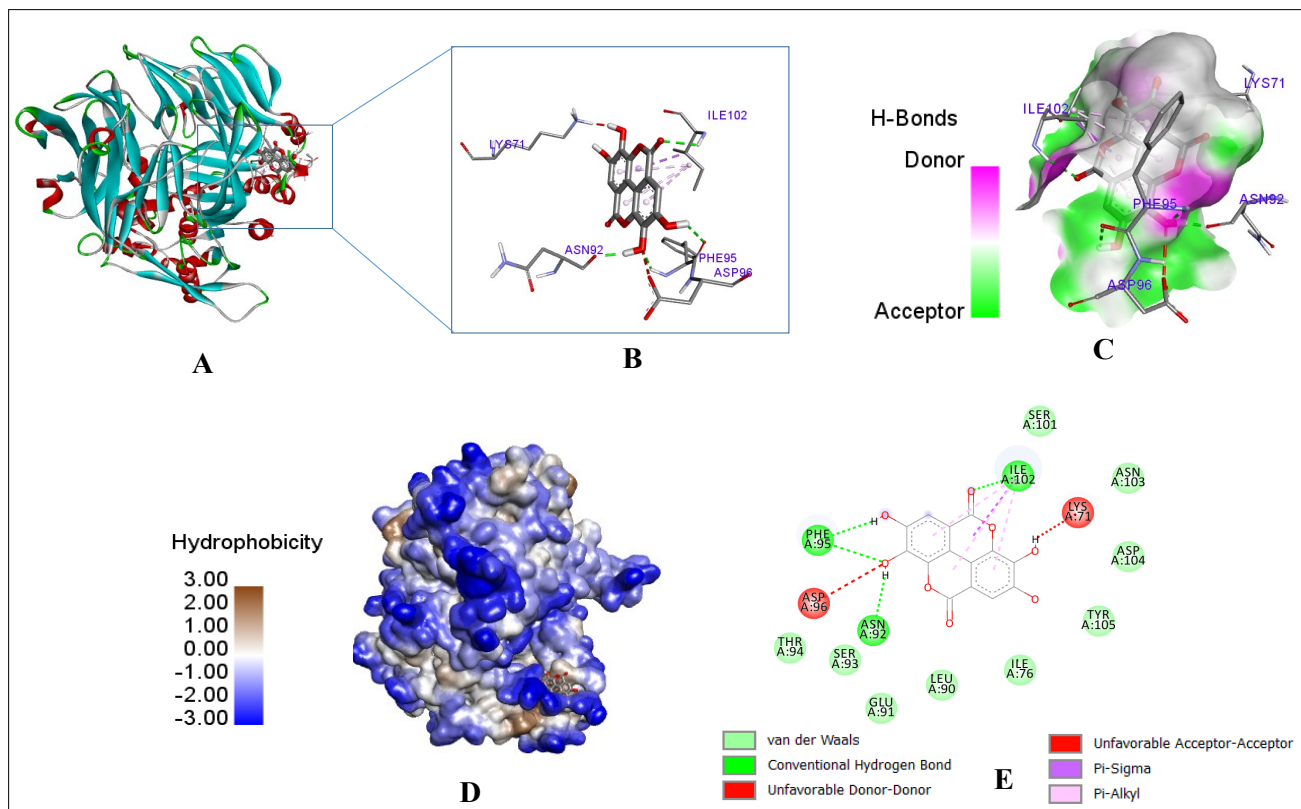


Fig. 3. 2D and 3D interaction diagram of ellagic acid with the active site residues of the human DPP4 protein (PDB ID:3W2T).

(A) Complex of DPP4 and ellagic acid; (B) Close view of pocket with ellagic acid; (C) Hydrogen bond donor and acceptor surface representation of the complex; (D) Hydrophobicity surface representation of the human DPP4 in complex with ellagic acid; (E) 2D representation of different types of interactions with ellagic acid

Ellagic acid interacts with DPP4 and forms hydrogen bonds with key residues ASN92, PHE95 and ILE102

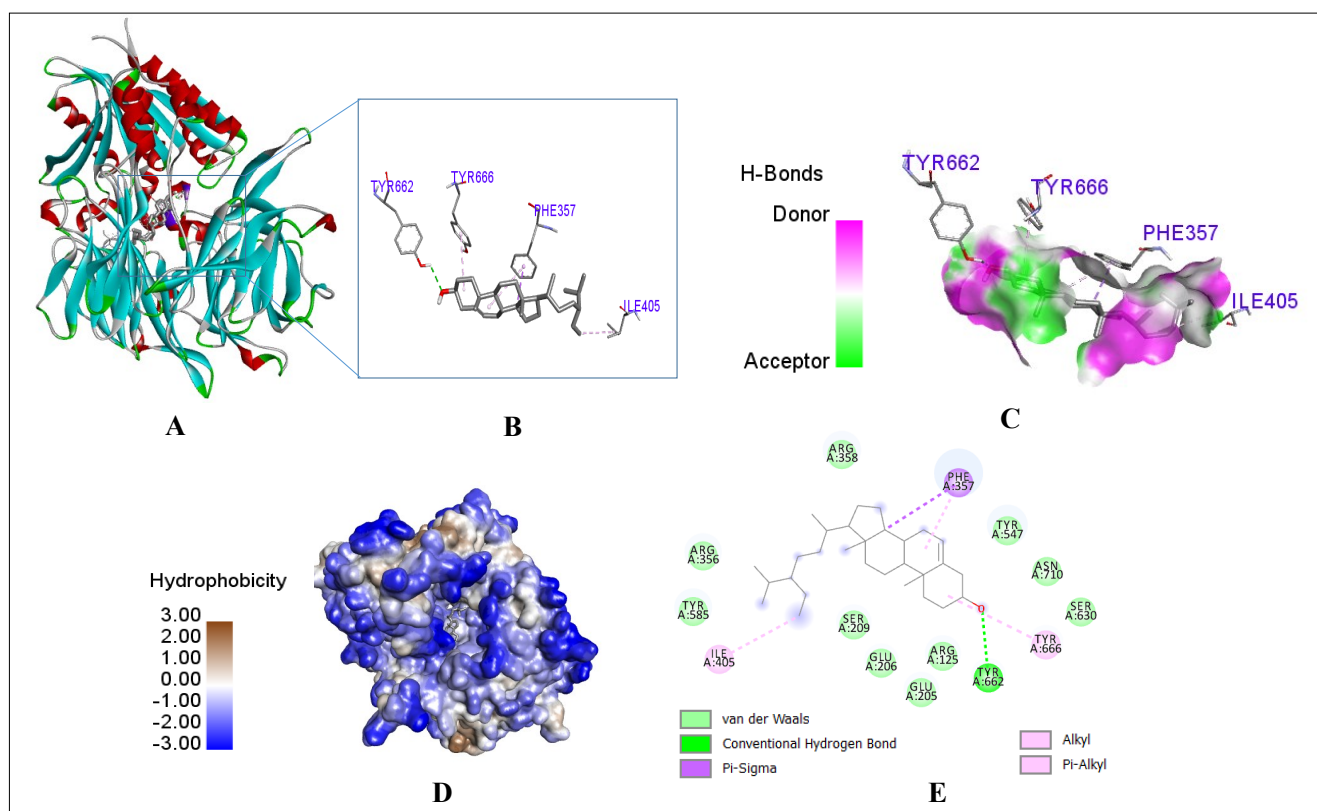


Fig. 4. 2D and 3D interaction diagram of β-sitosterol with the active site residues of the human DPP4 protein (PDB ID: 3W2T).

(A) Complex of DPP4 and β-Sitosterol; (B) Close view of pocket with β-sitosterol; (C) Hydrogen bond donor and acceptor surface representation of the complex; (D) Hydrophobicity surface representation of the human DPP4 in complex with β-sitosterol; (E) 2D representation of different types of interactions with β-Sitosterol.

β-Sitosterol forms hydrogen bond with key residue TYR 662 of the target protein DPP4

These interactions and their usefulness in T2DM need to be validated through experimental studies. In general, this study shows that in silico drug discovery has great potential to speed up identification of plant-based therapeutic leads and new ways of natural and cost-effective development of treatment against diabetes. In the coming decades, there is a possibility that phytomedicines could become a preferred treatment option for numerous diseases, including diabetes, over conventional drugs. The utilization of advanced scientific technologies and knowledge of traditional medicines can greatly contribute to the development of novel therapeutics.

Acknowledgements

The authors thank the management of Jagannath Majumder Research Foundation (JMRF), Tripura, India, for their support.

Authors' contributions

All authors contributed equally to the preparation of the manuscript. SM conceived the study. SM and GKP were involved in study design, data curation, molecular docking and manuscript writing. All authors read and approved the final manuscript.

Compliance with ethical standards

Conflict of interest: Authors have no conflict of interest to declare.

Ethical issues: None

References

- Deacon CF. Physiology and pharmacology of DPP-4 in glucose homeostasis and the treatment of type 2 diabetes. *Front Endocrinol.* 2019;10:80. <https://doi.org/10.3389/fendo.2019.00080>
- Makrilakis K. The role of DPP-4 inhibitors in the treatment algorithm of type 2 diabetes mellitus: when to select, what to expect. *Int J Environ Res Public Health.* 2019;16(15):2720. <https://doi.org/10.3390/ijerph16152720>
- Garg P, Duggal N. Type 2 diabetes mellitus, its impact on quality of life and how the disease can be managed-a review. *Obes Med.* 2022;35:100459. <https://doi.org/10.1016/j.obmed.2022.100459>
- Nistala R, Savin V. Diabetes, hypertension and chronic kidney disease progression: role of DPP4. *Am J Physiol Renal Physiol.* 2017;312:F661-F70. <https://doi.org/10.1152/ajprenal.00316.2016>
- Lee S, Lee H, Kim Y, Kim E. Effect of DPP-IV inhibitors on glycemic variability in patients with T2DM: a systematic review and meta-analysis. *Sci Rep.* 2019;9(1):13296. <https://doi.org/10.1038/s41598-019-49803-9>
- Bayanati M, Ismail Mahboubi Rabbani M, Sirous Kabiri S, Mir B, Rezaee E, Tabatabai SA. Dipeptidyl peptidase-4 inhibitors: a systematic review of structure-activity relationship studies. *Iran J Pharm Res.* 2024;23(1):e151581. <https://doi.org/10.5812/ijpr-151581>
- Duez H, Cariou B, Staels B. DPP-4 inhibitors in the treatment of type 2 diabetes. *Biochem Pharmacol.* 2012;83(7):823-32. <https://doi.org/10.1016/j.bcp.2011.11.028>
- Kaur S, Chaudhary R. A comprehensive review of the effects of *Psidium guajava* and *Syzygium cumini* leaves on diabetes mellitus. *Prev Nutr Food Sci.* 2025;30(3):209-21. <https://doi.org/10.3746/pnf.2025.30.3.209>
- Kumar S, Sharma S, Kumar V, Sharma A, Kaur R, Saini R. Jamun (*Syzygium cumini* (L.) Skeels): the conventional underutilized multifunctional plant-a view into its food and functional significance. *Ind Crops Prod.* 2023;191:115873. <https://doi.org/10.1016/j.indcrop.2022.115873>
- Hidayah H, Suherti I, Azzahra SS. Java Plum (*Syzygium cumini* (L.)) seeds potentials in medicinal uses: a systematic literature review. *Eureka Herba Indonesia.* 2023;4(2):221-6. <https://doi.org/10.37275/ehi.v4i2.72>
- Swami SB, Thakor NS, Patil MM, Haldankar PM. Jamun (*Syzygium cumini* (L.)): a review of its food and medicinal uses. *Food Nutr Sci.* 2012;3(8):1100-17. <https://doi.org/10.4236/fns.2012.38146>
- Chhikara N, Kaur R, Jaglan S, Sharma P, Gat Y, Panghal A. Bioactive compounds and pharmacological and food applications of *Syzygium cumini* - a review. *Food Funct.* 2018;9(12):6096-115. <https://doi.org/10.1039/C8FO00654G>
- Ahirwar R, Kumar S, Paradkar S, Singh S, Raghuwanshi S, Yadav S, et al. Phytochemical screening of jamun seed (*Syzygium cumini*). *Int J Sci Res Technol.* 2025.
- Das G, Nath R, Das Talukdar A, Sharma P, Kumar V, Singh R, et al. Major bioactive compounds from Java plum seeds: an investigation of its extraction procedures and clinical effects. *Plants (Basel).* 2023;12(6):1214.
- Jagetia GC. Phytochemical composition and pleiotropic pharmacological properties of jamun, *Syzygium cumini* Skeels. *J Explor Res Pharmacol.* 2017;2(2):54-66. <https://doi.org/10.14218/JERP.2016.00038>
- Kaur D, Yousuf B, Qadri OS. *Syzygium cumini* anthocyanins: recent advances in biological activities, extraction, stability, characterisation and utilisation in food systems. *Food Prod Process Nutr.* 2024;6(1):34. <https://doi.org/10.1186/s43014-023-00177-6>
- Panigrahi GK, Sahoo SK, Sahoo A, Behera S, Sahu SR, Dash A, et al. Bioactive molecules from plants: a prospective approach to combat SARS-CoV-2. *Adv Tradit Med.* 2023;1:14.
- Majumder S, Panigrahi GK. Molecular docking and ADME evaluation of plant-based bioactive molecules targeting nonsense-mediated mRNA decay pathway factors to modulate tumorigenesis. *Plant Sci Today.* 2024. <https://doi.org/10.14719/pst.3737>
- Pardo CG, Paranada JAR. Exploring the medicinal plants and traditional knowledge for common respiratory ailments among farmers in Ilocos Sur, Philippines. *Plant Sci Today.* 2025;12(3). <https://doi.org/10.14719/pst.7332>
- George BP, Chandran R, Abrahamse H. Role of phytochemicals in cancer chemoprevention: insights. *Antioxidants.* 2021;10:1455. <https://doi.org/10.3390/antiox10091455>
- Majrashi TA, Alshehri SA, Alsayari A, Muhsinah AB, Alrouji M, Alshahrani AM, et al. Insight into the biological roles and mechanisms of phytochemicals in different types of cancer: targeting cancer therapeutics. *Nutrients.* 2023;15(7):1704. <https://doi.org/10.3390/nu15071704>
- Zhou M, Konigsberg WH, Hao C, Pan Y, Sun J, Wang X. Bioactivity and mechanisms of flavonoids in decreasing insulin resistance. *J Enzyme Inhib Med Chem.* 2023;38(1):2199168. <https://doi.org/10.1080/14756366.2023.2199168>
- Poulose N, Prasad C, Haridas P, Anilkumar G. Ellagic acid stimulates glucose transport in adipocytes and muscles through AMPK mediated pathway. *J Diabetes Metab.* 2011;2(7):149. <https://doi.org/10.4172/2155-6156.1000149>
- Eid HM, Nachar A, Thong F, Sweeney G, Haddad PS. The molecular basis of the antidiabetic action of quercetin in cultured skeletal muscle cells and hepatocytes. *Pharmacogn Mag.* 2015;11(41):74. <https://doi.org/10.4103/0973-1296.149708>
- Ramalingam S, Packirisamy M, Karuppiiah M, Vasu G, Gopalakrishnan R, Gothandam K, et al. Effect of β -sitosterol on glucose homeostasis by sensitization of insulin resistance via enhanced protein expression of PPAR γ and glucose transporter 4 in high-fat diet and streptozotocin-induced diabetic rats. *Cytotechnology.* 2020;72(3):357

- 66. <https://doi.org/10.1007/s10616-020-00382-y>
26. Majumder S, Panigrahi GK. Advancements in contemporary pharmacological innovation: mechanistic insights and emerging trends in drug discovery and development. *Intell Pharm.* 2025;3(2):118-26. <https://doi.org/10.1016/j.ipha.2024.10.001>
 27. Jagetia GC. Bioactive phytoconstituents and medicinal properties of jamun (*Syzygium cumini*). *J Explor Res Pharmacol.* 2024;9(3):180-212.
 28. Raza A, Butt MS, Suleria HAR. Jamun (*Syzygium cumini*) seed and fruit extract attenuate hyperglycemia in diabetic rats. *Asian Pac J Trop Biomed.* 2017;7(8):750-4. <https://doi.org/10.1016/j.apjtb.2017.07.006>
 29. O'Boyle NM, Banck M, James CA, Morley C, Vandermeersch T, Hutchison GR. Open Babel: an open chemical toolbox. *J Cheminform.* 2011;3(1):33. <https://doi.org/10.1186/1758-2946-3-33>
 30. Morris GM, Huey R, Lindstrom W, Sanner MF, Belew RK, Goodsell DS, et al. AutoDock4 and AutoDockTools4: automated docking with selective receptor flexibility. *J Comput Chem.* 2009;30(16):2785-91. <https://doi.org/10.1002/jcc.21256>
 31. Trott O, Olson AJ. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function. *J Comput Chem.* 2009;31:455-61. <https://doi.org/10.1002/jcc.21334>
 32. Daina A, Michielin O, Zoete V. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Sci Rep.* 2017;7:42717. <https://doi.org/10.1038/srep42717>
 33. Lipinski CA. Lead- and drug-like compounds: the rule-of-five revolution. *Drug Discov Today Technol.* 2004;1(4):337-41. <https://doi.org/10.1016/j.ddtec.2004.11.007>
 34. Ganguly G, Hussain A, Nayak A. In silico evaluation of DPP-4 inhibitors: a comparative docking approach. *SSRN*; 2025. <https://doi.org/10.2139/ssrn.5284350>
 35. Saraiva AA, Soares JN, Costa NJ, Sousa JV, Ferreira NM, Valente A, et al. Study of dipeptidil peptidase 4 inhibitors based on molecular docking experiments. In: *INBIOINFORMATICS 2019*; 322-30. <https://doi.org/10.5220/0007692203220330>