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In-silico screening of Alpha Amylase Enzyme Inhibitors from Siddha Formulation *Pungampoo Chooranam* by Molecular docking analysis for the management of Type II Diabetes mellitus

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Abstract

Diabetes Mellitus is a major health care problem in India with prevalence of about 66.8 million and it was expected to reach 80 million by the year 2025. Type II diabetes (T2DM) accounts for the majority of all diagnosed cases of diabetes in the world with its prevalence increasing sharply in recent decade.The inhibition of alpha-amylase an enzyme involved in the digestion of carbohydrates, can significantly reduce the post-prandial increase of blood glucose and therefore can be an important strategy in the management of blood glucose level in type II diabetic and borderline patients. The main aim of the present investigation is to screen the alpha amylase enzyme inhibition potential of novel phytocomponents such as Beta Sitosterol, Glabrin, Isolonchocarpin, Kanjone, Pongol, Sterolin, Pinnatin and Quercetin present in the formulation *Pungampoo Chooranam* (PPC) against target protein alpha amylase receptor with PDB code 1HNY along with the standard acarbose using computational docking analysis. The results of the study indicate that the lead pinnatin has shown highest inhibition property similar to that of the standard acarbose. The second highest docking interaction possessed by beta sitosterol followed by this Isolonchocarpin, kanjone , pongol and quercetin. The leads such as glabrin and sterolin has no interaction with any of the significant amino acid residues on the target alpha amylase. Based on the results of the In-silico screening analysis it was concluded that the compound's such as pinnatin, beta sitosterol , Isolonchocarpin, kanjone ,pongol and quercetin present in the siddha formulation PPC may possess significant anti-diabetic property by inhibition of target enzyme alpha amylase.

Keywords: Diabetes Mellitus, *Pungampoo Chooranam*, alpha amylase, anti-diabetic, Beta Sitosterol, Glabrin, Isolonchocarpin, Kanjone, Pongol, Sterolin, Pinnatin, Quercetin

1. Introduction

Diabetes is multifactorial and has been associated with various disorders including obesity, dyslipidemia, thrombosis, infarction, hypertension, endothelial dysfunction, and coronary artery disease. The global prevalence of diabetes mellitus is forecast to reach 300 million by 2025, and over three quarters of the deaths amongst this population will be expected to result from cardiovascular disease [1]. Individuals with diabetes are at a significantly greater risk of developing both micro- and macrovascular disease and have a cardiac mortality equivalent to that in nondiabetic patients with confirmed heart disease [2].

Type II diabetes is one of the primary threats to human health due to increasing prevalence, chronic course and disabling complications [3]. Many diverse therapeutic strategies for the treatment of Type II diabetes are in use. The conventional available therapies for diabetes include stimulation of endogenous insulin secretion, enhancement of the action of insulin at the target tissues, oral hypoglycemic agents, such as biguanids and sulfonylureas and the inhibition of degradation of dietary starch by glycosidases such as α-amylase and α-glucosidase [4].

Pancreatic α-amylase inhibitors offer an effective strategy to lower the levels of post-prandial hyperglycemia via control of starch breakdown. Pancreatic α-amylase is a key enzyme in the digestive system and catalyses the initial step in hydrolysis of starch to a mixture of smaller oligosaccharides consisting of maltose, maltotriose, and a number of α-(l-6) and α-(1 - 4) oligoglucans. These are then acted on by α-glucosidases and further degraded to glucose which on absorption enters the blood-stream.

Indian medicinal plants used in the siddha system of traditional medicine to treat diabetes become a potential source of novel anti-diabetic agents. The primary healthcare benefits of using plant-derived siddha formulations are relatively safer when compared to allopathic drugs and offer profound therapeutic benefits [5]. Single and polyherbal preparations have diverse range of bioactive molecules and play a dominant role in the maintenance of human health since ancient times [6]. More than 1500 herbal preparations are sold as dietary supplements or ethnic traditional medicines [7].

Pongamia pinnata (Fabaceae) is popularly known as Indian beech in English [8]. Commonly known by its vernacularnames karanj (Hindi), honge/karajata (Kannada), pungai (Tamil). As per the literature the extract of stem bark of *P. pinnata* (L.) showed antihyperglycaemic activity in diabetic mice [9]. Further, reports available that concomitant administration of synthetic oral hypoglycemic drugs along with *P. pinnata* produced synergistic effect in diabetic mice[10]. The preliminary phytochemical analysis showed the presence of alkaloids, terpenoids, triterpenes, flavonoids, steroids, and volatile oils [11]. It has been identified that Cycloart-23-ene-3*β*, 25-diol (B2) isolated from the stem bark of *P. pinnata* possesses antidiabetic activity in diabetic animals [12, 13]. Cycloart-23-ene-3*β*, 25-diol improved the abnormalities of diabetic conditions in diabetic mice due to increased glucagon-like peptide 1 (GLP-1) insulin secretion [14] and has a protective effect on vital organs like heart and kidney [15].

Computer aided drug discovery attains greater importance mainly because of the reliability in the results and also paves a new way for the research focus towards the alternative animal models. Molecular Docking continues to hold great promise in the field of Computer based drug design that screens small molecules by orienting and scoring them in the binding site of a protein. As a result novel ligands for receptors of known structure were designed and their interaction energies were calculated using the scoring functions. Dock score was used to estimate the ligand-binding energies. Apart from these, other input parameters for docking are also considered for evaluating the compounds inhibition efficacy. It is estimated that docking programs currently dock 70 – 80% of ligands correctly [16]. The main aim of the present investigation is to screen the anti-diabetic potential of phytocomponents

such as Beta Sitosterol, Glabrin, Isolonchocarpin, Kanjone, Pongol, Sterolin, Pinnatin and Quercetin present in the formulation *Pungampoo Chooranam* (PPC) against target protein alpha amylase receptor with PDB code 1HNY along with the standard acarbose using auto-dock computational docking analysis.

2. Materials and Methods

2.1. Source of raw drugs:

The herb is collected from southern zone of Tamil Nadu, and other required ingredient is procured from a well reputed indigenous drug shop from Parrys corner, Chennai, Tamil Nadu, India .Herb were authenticated by the Pharmacognosist, SCRI Chennai, Tamil Nadu, India

2.2. Ingredients

The siddha formulation *Pungampoo Chooranam* (PPC) comprises of two main ingredients as listed below

1. Pungam flowers (*Pongamia pinnata*)
2.Cow's Ghee

2.3.Preparation [17]

The shade dried flowers of *Pongamia pinnata* were roasted slowly by adding little bit of cow's ghee. Then it is powdered and sieved using cloth.

Dosage : 2 gm twice a day
Adjuvant : Warm water
Duration : 48 Days

2.4. Software's required

Several docking tools were been used in recent times which works behind structure-based drug design strategies one among which is auto dock a componential software tools used to analyze the protein 1HNY and to study the binding energy properties with the following lead component such as Beta Sitosterol, Glabrin, Isolonchocarpin, Kanjone, Pongol, Sterolin, Pinnatin and Quercetin along with standard Acarbose. Human alpha amylase receptor with PDB code 1HNY was obtained from protein data bank (www.pdb.org/pdb/). To get insight the intermolecular interactions, the molecular docking studies were done for the above mentioned phytoconstituents along with standard at the active site 3D space of enzyme of interest alpha amylase using online DOCKING SERVER web tool module.

2.5. Ligand preparation

The ligands such as Beta Sitosterol, Glabrin, Isolonchocarpin, Kanjone, Pongol, Sterolin, Pinnatin and Quercetin along with standard Acarbose built using Chemsketch and optimized using Docking server online web tool as shown in Figure 1 and 2 for docking studies by using Geometry optimization method MMFF94 and charge calculation was carried out based on Gasteiger method at PH 7 as shown in Table 1.

Table 1: Ligand Properties of the selected Lead

S.No	Name of the Compounds	Molar weight g/mol	Molecular Formula	H Bond Donor	H Bond Acceptor	Rotatable bonds	Log P
1	Beta Sitosterol	414.718 g/mol	C29H50O	1	1	6	9.3
2	Acarbose	645.608 g/mol	C25H43NO18	14	19	9	-8.5
3	Glabrin	175.184 g/mol	C7H13NO4	3	5	1	-3.5
4	Isolonchocarpin	306.361 g/mol	C20H18O3	0	3	1	3.8
5	Kanjone	292.29 g/mol	C18H12O4	0	4	2	3.6
6	Pongol	292.29 g/mol	C18H12O4	0	4	2	3.6
7	Sterolin	576.859 g/mol	C35H60O6	4	6	9	7.7
8	Pinnantin	292.29 g/mol	C18H12O4	0	4	2	3.6
9	Quercetin	302.238 g/mol	C15H10O7	5	7	1	1.5

Fig 1: 2D Structure of lead 1.Beta Sitosterol 2.Glabrin 3.Isolonchocarpin 4.Kanjone 5.Pongol 6.Sterolin 7. Pinnatin 8.Quercetin and 9.Acarbose

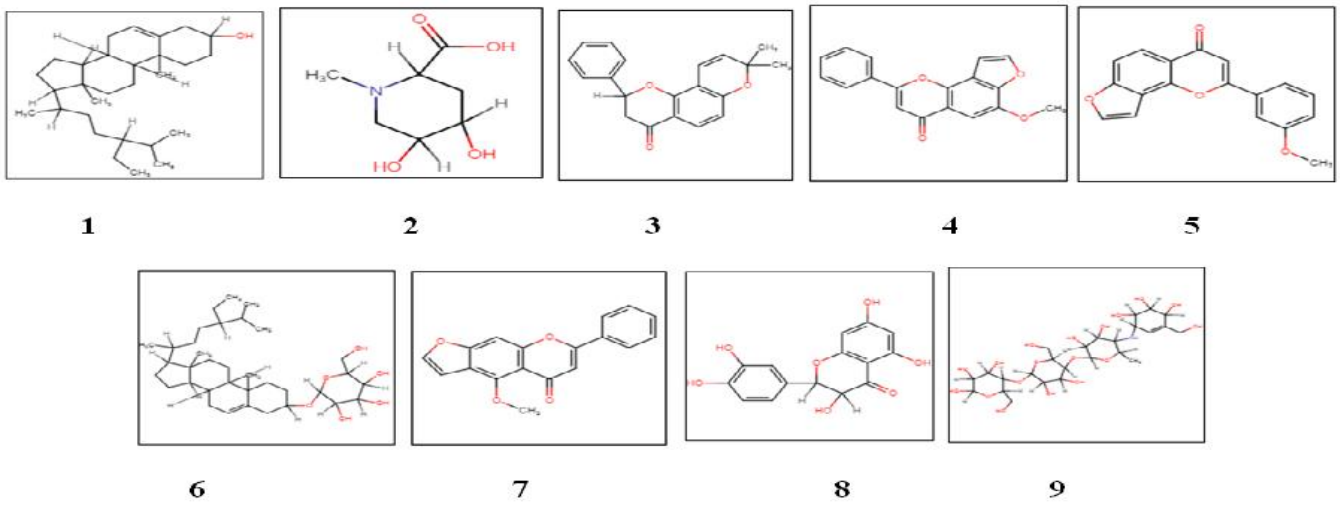
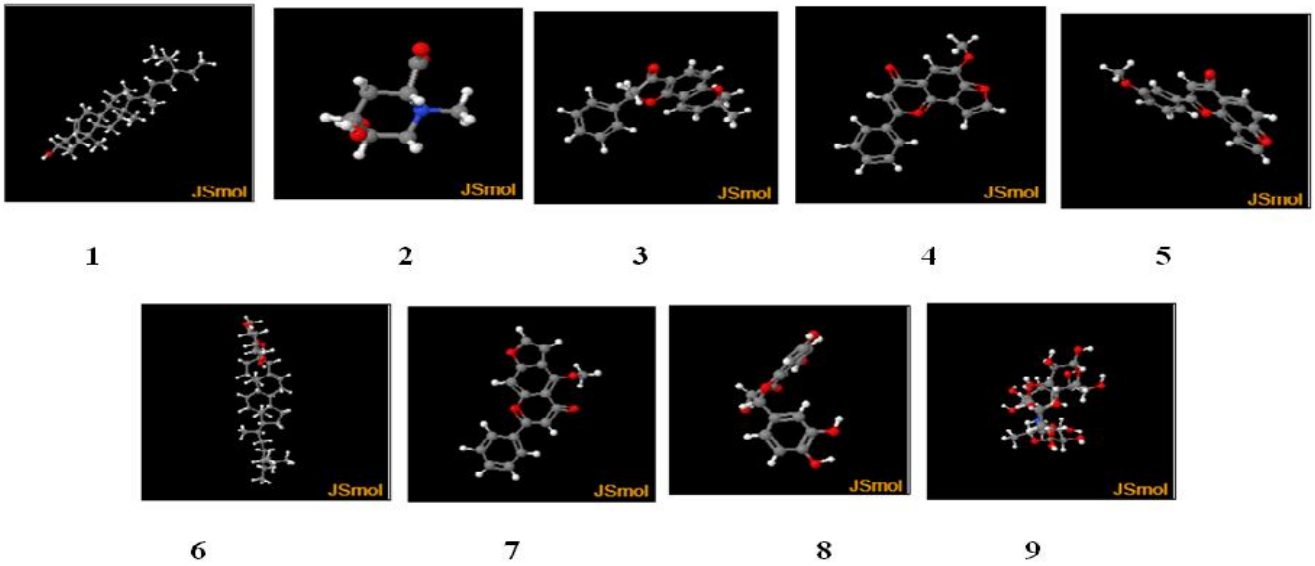


Fig 2: 3D Structure of lead 1.Beta Sitosterol 2.Glabrin 3.Isolonchocarpin 4.Kanjone 5.Pongol 6.Sterolin 7. Pinnatin 8.Quercetin and 9.Acarbose



2.5. Active Site Prediction

Active site of enzyme was obtained by LIGSITE web server by using the automatic identification of pockets on protein surface given 3D coordinates of protein. The potential ligand binding sites in 1HNY target protein is identified using grid space of 1 and probe of radius 5.0 angstrom [18]. Ligand site prediction was performed by using online tool GHECOM and the respective pockets calculations [19,20].

2.6. Docking Methodology

Docking calculations were carried out using Docking Server [21,22]. Gasteiger partial charges were added to the ligand atoms. Non-polar hydrogen atoms were merged, and rotatable bonds were defined. Docking calculations were carried out based on the binding free energy on the following compounds like Beta Sitosterol, Glabrin, Isolonchocarpin, Kanjone, Pongol, Sterolin, Pinnatin and Quercetin along with standard Acarbose and their binding affinity towards the target protein with PDB 1HNY as shown in figure 3.

Fig 3:Target protein Alpha amylase receptor with PDB code 1HNY

Essential hydrogen atoms, Kollman united atom type charges, and solvation parameters were added with the aid of Auto Dock tools. Affinity (grid) maps of Å grid points and 0.375 Å spacing were generated using the Autogrid program. Auto Dock parameter set and distance-dependent dielectric functions were used in the calculation of the van der Waals and the electrostatic terms, respectively. Docking simulations were performed using the Lamarckian genetic algorithm (LGA) and the Solis and Wets local search method [23]. Initial position, orientation, and torsions of the ligand molecules were set randomly. All rotatable torsions were released during docking. Each docking experiment was derived from 2 different runs that were set to terminate after a maximum of 250000 energy evaluations. The population size was set to 150.

During the search, a translational step of 0.2 Å, and quaternion and torsion steps of 5 were applied [24].

3. Results

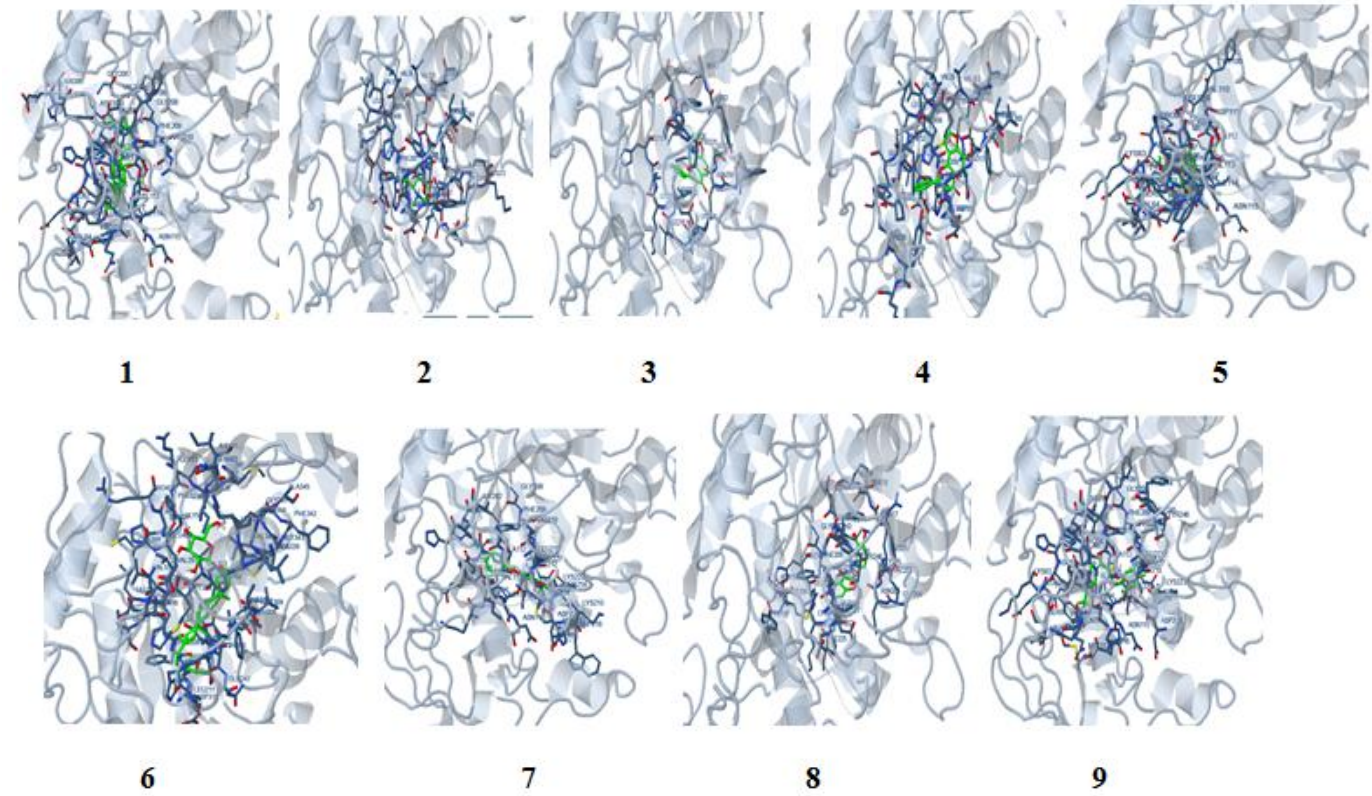
3.1. Dock scores

The result of binding interactions of the ligand with alpha amylase has revealed that out of eight compounds docked against PDB 1HNY.The lead pinnatin has shown highest inhibition property similar to that of the standard acarbose. The second highest docking interaction possessed by beta sitosterol followed by this Isolonchocarpin, kanjone , pongol and quercetin. The leads such as glabrin and sterolin has no interaction with any of the significant amino acid residues on the target alpha amylase as shown in table 2 and fig 4.

Table 2: Summary of the molecular docking studies of compounds against Alpha amylase receptor

S.No	Name of the Compounds	Binding Free energy Kcal/mol	Inhibition constant Ki µM (*mM)	Electrostatic energy Kcal/mol	Intermolecular energy Kcal/mol	Total Interaction Surface
1	Beta Sitosterol	-8.18	1.01	-0.01	-9.67	807.19
2	Acarbose	-9.34	143.4*	-0.05	-11.23	802.44
3	Glabrin	-4.26	752.7	-0.95	-5.32	393.48
4	Isolonchocarpin	-6.25	26.27	-0.31	-8.83	753.68
5	Kanjone	-6.22	27.38	-0.11	-8.95	909.2
6	Pongol	-5.98	41.69	-6.42	-6.55	570.38
7	Sterolin	-8.55	540.42*	-0.05	-10.75	1081.66
9	Pinnantin	-5.73	63.56	-0.13	-6.29	627.76
10	Quercetin	-6.25	26.20*	-0.38	-6.8	591.56

Fig 4 : Possible ligand binding pockets on the surface of target Alpha amylase receptor with PDB code 1HNY. Pockets calculated by GHECOM.



3.2 Amino acid interaction Study

The core amino acids responsible for alpha amylase enzyme activity was found to be Trp 58, Trp 59, Tyr 62, His 101, Leu 162, Arg 195, Asp 197, Ala 198, Ser 199, Lys 200, His 201, Glu 233, Asp 300.It was observed from the present investigation that the lead molecules such as pinnatin, beta sitosterol, Isolonchocarpin, kanjone ,pongol and quercetin has a tendency to interact with above mentioned amino acid residues responsible for enzyme inhibition potential of the formulation PPC. The results were shown in table 3.

Table 3: Interaction of lead compounds with active site amino acid residue of Alpha amylase Receptor

Compound	Amino Acid Interaction													
Beta Sitosterol	59 PRO	60 PRO	61 ASN	63 ASN	79 PRO	94 PHE	110 VAL	112 ALA	113 VAL	114 ILE	197 TYR	198 MET	201 LEU	202 ILE
Acarbose	59 PRO	61 ASN	79 PRO	82 TYR	110 VAL	111 ASP	112 ALA	113 VAL	114 ILE	116 HIS	194 ILE	197 TYR	198 MET	201 LEU
Glabrin	30 HIS	56 GLN	111 ASP	210 ARG	248 GLU	269 THR	271PHE	310 PHE	313 ASN	314 HIS	314 HIS	315 ASP	352 ARG	
Isolonchocarpin	59 PRO	60 PRO	61 ASN	63 ASN	79 PRO	82 TYR	110 VAL	111 ASP	112 ALA	113 VAL	114 ILE	197 TYR	201 LEU	209 PHE
Kanjone	30 HIS	32 PHE	56 GLN	58 SER	59 PRO	77 TYR	111 ASP	210 ARG	310 PHE	313 ASN	314 HIS	352 ARG	354 MET	
Pongol	59 PRO	60 PRO	61 ASN	63 ASN	76 ARG	79 PRO	82 TYR	110 VAL	112 ALA	113 VAL	114 ILE	194 ILE	197 TYR	
Sterolin	30 HIS	56 GLN	210 ARG	246 TYR	248 GLU	269 THR	271 PHE	310 PHE	311 VAL	312 ASP	313 ASN	314 HIS	315 ASP	336 TYR
Pinnatin	112 ALA	114 ILE	194 ILE	197 TYR	198 MET	201 LEU	209 PHE	211 LEU	214 SER	217 MET	222 ILE	225 ILE	226 LEU	
Quercetin	17 TYR	198 MET	209 PHE	211 LEU	226 LEU	229 LEU	242 LYS	243 PRO	244 PHE	245 ILE				

4. Discussion

Diabetes is multifactorial and has been associated with various disorders including obesity, dyslipidemia, thrombosis, infarction, hypertension, endothelial dysfunction, and coronary artery disease [25]. However, diastolic and systolic dysfunctions are mainly altered apart from traditional cardiac risks parameters such as hypertension, atherosclerosis, and dyslipidemia [26]. Diabetic patients have an increased risk of cardiovascular diseases and these are the major cause of death in them [27, 28]. Cardiomyopathy is a prevalent cause of death in patients with diabetes [29]. The world prevalence of diabetes among adults (aged 20–79 years) will be 6.4%, affecting 285 million adults, in 2010 and will increase to 7.7%, affecting 439 million adults, by 2030 [30,31].

Search of alternate therapy from the natural origin is a never ending process in this view herbs become the predominant source for the supply of valuable therapeutic leads with multiple components and may render versatile pharmacological action against several diseases in recent times. Use of plants as a source of medicine has been inherited and is an important component of the health care system. India is the largest producer of medicinal herbs and is appropriately called the botanical garden of the world [32]. Plants used for traditional medicine contain a wide range of substances that can be used to treat chronic as well as infectious diseases [33].

Siddha system of medicine become popular throughout the world in recent days as it claims high curative value with minimum toxicity and have less side effects. It has been estimated that 70-80% of world's population relies on traditional healthcare. The mode of preparation and plant used in traditional medicine varies from place to place. In addition acceptance of traditional medicines, especially herbal medicines in the developed world is sharply increasing [34].

Molecular docking has become an increasingly important tool for drug discovery. In this review, we present a brief introduction of the available molecular docking methods, and their development and applications in drug discovery. The relevant basic theories, including sampling algorithms and scoring functions, are summarized. The differences in and performance of available docking software are also discussed. Flexible receptor molecular docking approaches, especially those including backbone flexibility in receptors, are a challenge for available docking methods [35].

The result of binding interactions of the ligand with alpha amylase has revealed that out of eight compounds docked against PDB 1HNY.The lead pinnatin has shown highest inhibition property similar to that of the standard acarbose. The second highest docking interaction possessed by beta sitosterol followed by this Isolonchocarpin, kanjone , pongol and quercetin. The leads such as glabrin and sterolin has no interaction with any of the significant amino acid residues on the target alpha amylase.

The molecular docking approach can be used to model the interaction between a small molecule and a protein at the atomic level, which allow us to characterize the behavior of small molecules in the binding site of target proteins as well as to elucidate fundamental biochemical processes [36].The docking process involves two basic steps: prediction of the ligand conformation as well as its position and orientation within these sites (usually referred to as *pose*) and assessment of the binding affinity. These two steps are related to sampling methods and scoring schemes, respectively, which will be discussed in the theory section.

5. Conclusion

From the results of the In-silico screening analysis it was concluded that the compound's such as pinnatin, beta sitosterol, Isolonchocarpin, kanjone ,pongol and quercetin present in the siddha formulation *Pungampoo Chooranam* (PPC) may possess significant anti-diabetic property by inhibition of target enzyme alpha amylase. It is evident that effective inhibition of the enzyme pancreatic α-amylase offers an effective strategy

to lower the levels of post-prandial hyperglycemia via control of starch breakdown. Hence it was concluded that the formulation.

PPC may be used for the clinical management of T2DM because of its biologically significant phytotherapeutics which acts synergistically by inhibiting the key enzymes involved in the regulation of blood glucose level.

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References

1. King H, Aubert RE, Herman WH. Global burden of diabetes, 1995–2025: prevalence, numerical estimates, and projections. Diabetes Care. 1998; 21(9):1414–1431.
2. Murarka S, Movahed MR. Diabetic cardiomyopathy. Journal of Cardiac Failure. 2010;16:971–979.
3. Leena AA, Jill PC. Type II Diabetes Prevention: A Review. Clinical Diabetes. 2010; 28:53–59.
4. Rang HP, Dale MM, Ritter JM, Moore PK. Pharmacology. 5. Churchill Livingstone; 2003:382.
5. Barrett B, Kiefer D, Rabago D. Assessing the risk and benefits of herbal medicine: An overview of scientific evidence. Alter Health Med. 1999;5:40–49.
6. Handa SS. Indian efforts for quality control and standardization of herbal drugs and products. Proceedings of the 1st joint workshop on quality control and standardization of traditional medicine–Indo-China experience. 2004.
7. WHO. General guidelines for methodologies on research and evaluation of traditional medicine. Geneva: World Health Organization; 2000.
8. Krishnamurthi A. The Wealth of India—Raw Materials: Ph-Re. Vol. 8. New Delhi, India: Publication and Information Directorate, Council of Scientific and Industrial Research; 1998.
9. Badole SL, Bodhankar L. Antihyperglycemic activity of Pongamia pinnata stem bark in diabetic mice. Pharmaceutical Biology. 2008;46:900–905.
10. Badole SL, Bodhankar SL. Investigation of antihyperglycaemic activity of aqueous and petroleum ether extract of stem bark of *Pongamia pinnata* on serum glucose level in diabetic mice. Journal of Ethnopharmacology. 2009;123:115–120.
11. Badole SL, Bodhankar SL. Concomitant administration of petroleum ether extract of the stem bark of Pongamia pinnata (L.) Pierre with synthetic oral hypoglycaemic drugs in alloxan-induced diabetic mice. European Journal of Integrative Medicine. 2009;1:73–79.
12. Badole SL, Bodhankar SL. Antihyperglycaemic activity of cycloart-23-ene-3β, 25-diol isolated from stem bark of Pongamia pinnata in alloxan induced diabetic mice. Research Journal of Phytochemistry. 2009;3:18–24.
13. Badole SL, Bodhankar SL. Antidiabetic activity of cycloart-23-ene-3β, 25-diol (B2) isolated from Pongamia pinnata (L. Pierre) in streptozotocin-nicotinamide induced diabetic mice. European Journal of Pharmacology. 2010;632:103–109.

14. Badole SL, Bagul PP, Mahamuni SP. Oral L-glutamine increases active GLP-1 (7-36) amide secretion and improves glycemic control in stretpozotocin-nicotinamide induced diabetic rats. Chemico-Biological Interactions. 2013;203:530–541.
15. Badole SL, Bodhankar SL, Raut CG. Protective effect of cycloart-23-ene-3β, 25-diol (B2) isolated from Pongamia pinnata L. Pierre on vital organs in streptozotocin-nicotinamide induced diabetic mice. Asian Pacific Journal of Tropical Biomedicine. 2011;1:186–190.
16. Sivaraman D, Panneerselvam P. Screening of Potential Glycogen synthase kinase -3β inhibitors from Herbal lead by In-Silico Docking Technique. International journal of Chem Tech research.2015;08:834-842.
17. Boga Munivar .Boga Munivar Vaithiyam 700.B. Rathina Nayakkar & Sons.2012. Seiyul no:199, 200.
18. Bingding H, Michael S. Schroeder "LIGSITE ^{csc}: Predicting protein binding sites using the Connolly surface and degree of conservation. BMC structural Biology.2006;6:01-11.
19. Kawabata T. Detection of multi-scale pockets on protein surfaces using mathematical morphology. Proteins.2010;78:1195-1121.
20. KawabataT. Detection of pockets on protein surfaces using small and large probe spheres to find putative ligand binding sites. Proteins.2007; 68:516-529.
21. Bikadi Z, Hazai E. Application of the PM6 semi-empirical method to modeling proteins enhances docking accuracy of AutoDock. J. Cheminf.2009;1:15.
22. Halgren TA. Molecular force field. I. Basis, form, scope, parametrization, and performance of MMFF94.J Comput Chem.1998;17:490-519.
23. Morris GM. Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function .J Comput Chem.1998;19:1639-1662.
24. Solis FJ. Minimization by Random Search Techniques. Mathematics of Operations Research.1981;6:19-30.
25. Maya L, Villarreal FJ. Diagnostic approaches for diabetic cardiomyopathy and myocardial fibrosis. Journal of Molecular and Cellular Cardiology. 2010;48:524–529.
26. Wang J, Song Y, Wang Q, Kralik PM, Epstein PN. Causes and characteristics of diabetic cardiomyopathy. The Review of Diabetic Studies. 2006;3:108–117.
27. Zhi YF, Prins JB, Marwick TH. Diabetic cardiomyopathy: evidence, mechanisms, and therapeutic implications. Endocrine Reviews. 2004;25:543–567.
28. Kannel WB, Hjortland M, Castelli WP. Role of diabetes in congestive heart failure: the Framingham study. The American Journal of Cardiology. 1974;34:29–34.
29. Boudina S., Abel E. D. Diabetic cardiomyopathy revisited. Circulation. 2007;115:3213–3223.
30. Sulaiman M, Matta MJ, Sunderesan NR. Resveratrol, an activator of SIRT1, upregulates sarcoplasmic calcium ATPase and improves cardiac function in diabetic cardiomyopathy. American Journal of Physiology—Heart and Circulatory Physiology. 2010,298:833–843.
31. Shaw JE, Sicree RA, Zimmet PZ. Global estimates of the prevalence of diabetes for 2010 and 2030. Diabetes Research and Clinical Practice. 2010;87:4–14.
32. Ahmedull M, Nayar MP. Red data book for Indian plants, Botanical Survey of India. vol. 4. Calcutta: 1999.
33. Duraipandiyan V, Ayyanar M, Ignacimuthu S. Antimicrobial activity of some ethnomedicinalplants used by Paliyar tribe from Tamil Nadu, India. BMC Complement Altern Med. 2006;6:35–41.
34. Bharathi Sri R. Shanmugapriya.C, Meenakumari R. Formulation, Standardization and Physiochemical Evaluation Of Siddha Formulation Poovarasu Nei By Modern Analytical Techniques.WJPPS.2017;6: 991-1008
35. Xuan-Yu Meng. Molecular Docking: A powerful approach for structure-based drug discovery. Curr Comput Aided Drug Des. 2011 ; 7: 146–157.

36. McConkey BJ, Sobolev V, Edelman M. The performance of current methods in ligand-protein docking. Current Science. 2002; 83:845–855.

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