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Research Article

TYPE 2 DIABETES: INTERACTION BETWEEN CINNAMONPOLYPHENOL AND HUMAN SERUM PROTEIN

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ABSTRACT

Cinnamonpolyphenol acts on human serum protein.The human serum albumin in turn switches on the gene in the islet of langerhans in the pancreas which induces the beta cells to produce insulin. This helps to lower the sugar levels in Type 2 diabetic patients. The interaction between cinnamonpolyphenol and human serum protein has been studied in detail using the autodock software. Cinnamonpolyphenol binds to the human serum protein and the docking energy for the process was recorded to be -3.60 kcal/mol.

Keywords: Diabetic, Cinnamonpolyphenol, Docking

INTRODUCTION

Diabetes has been one of the most prevalent condition in Asian pacific region. There are two types of diabetes Type 1 and Type 2.Among these type 2 has been considered as chronic progressive state. During this state the plasma glucose rises gradually in spite of the type of treatment [7].

Type 2 diabetes is one of the major public health concerns in both developing and developed countries in the Asian-Pacific region. It has become epidemic in a number of countries, particularly in newly industrialized nations. Healthcare budgets of many countries have been affected as a result of the direct and indirect social and economic costs of treating diabetes and its complications.

Type 2 diabetes results in the following symptoms premature morbidity and mortality, particularly from cardiovascular disease (CVD), blindness, amputations and renal failure. Also it is a part of the metabolic syndrome, a cluster of major CVD risk factors previously also referred to as the insulin resistance syndrome, Syndrome X or the Deadly Quartet [6].

Cinnamon has been long known for its medicinal as well as its ability to enhance taste of food. Researchers have studied the effect of various compounds present in cinnamon on the sugar level of type 2 diabetic patients. These compounds include cinnamonaldehyde, cinnamonnitrile and cinnamonpolyphenol. The interaction of cinnamonpolyphenol and human serum protein at the molecular level is studied in this paper.

Cinnamonpolyphenol displays insulin like properties as well as enhances glucose metabolism [1]. Cinnamon and its components improve blood glucose, lipids, and insulin function in animals. The effect of cinnamon was studied in rats. The effect was seen in rats fed with high fructose diet. They showed an elevated blood glucose level and insulin resistance was reduced by the administration of whole cinnamon or an aqueous extract of cinnamon. The active components of cinnamon include type A polymers, one tetramer and four type A trimers have been isolated from cinnamon and all were shown to have in vitro insulin-potentiating activity. Cinnamon treated rats showed significantly higher glucose metabolism rates compared to controls [2].

Several phenolic compounds found in cinnamon, such as catechin, epicatechin, procyanidin B2 and phenol polymers, all showed significant inhibitory effects on the formation of advanced glycation end products [3]. Their antiglycation activities are not only brought about by their antioxidant activities, but are also related to the trapping abilities of reactive carbonyl species. The study demonstrated that proanthocyanidins can effectively scavenge reactive carbonyl species, inhibit the formation of advanced glycation end products, and, therefore, have the potential to be developed as agents to alleviate diabetic complications [4]. Cinnamon extracts are reported to have beneficial effects on people with normal and impaired glucose tolerance, the metabolic syndrome, type 2 diabetes and insulin resistance [5].

MATERIALS AND METHODS

Chemsketch

Chemsketch is a freeware software used primarily to design molecules [9]. In addition it could be used to calculate various physical properties of the molecule. The structure of cinnamonpolyphenol was designed using the molecular design software chemsketch. The structure includes benzene rings as well as hydroxyl group as residues.

Protein data bank

Protein data bank (PDB) is a repository for 3-D structure of protein and which studies various proteins in detail. The 3-D file of human serum protein was obtained from PDB. The protein consists of two chains.

Autodock

Autodock is a docking and simulation software particularly used to study the interaction of ligand and receptor molecules. This docking and simulation software was used to load the ligand as well as the protein files and to study the interaction between cinnamonpolyphenol and human serum protein [8].

RESULT AND DISCUSSIONS

The ligand compound cinnamonpolyphenol was sketched in chemsketch (Fig 1).

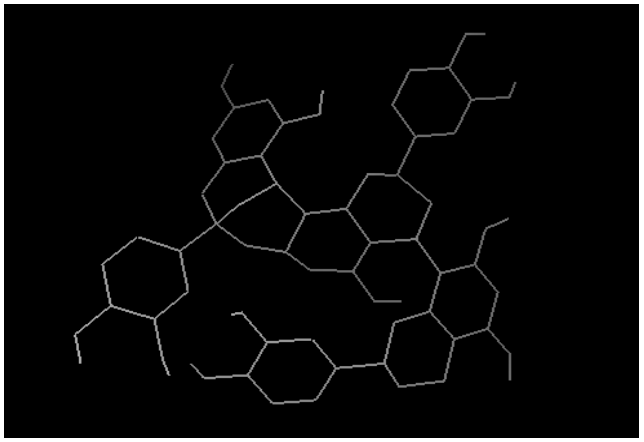

Fig. 1: Cinnamonpolyphenol in Chemsketch

The human serum protein pdb file was obtained from PDB (Fig 2).The protein consists of two chains A and L. Structural details of

Human serum albumin was obtained from PDB and studied in detail in Argus lab.

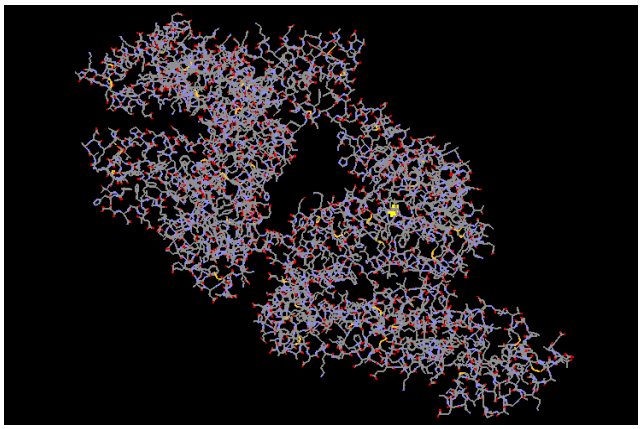

Fig. 2: The pdb file of human seum albumin

Docking of the ligand and the protein files was carried out by autodock. It was observed cinnamonpolyphenol compound binds to the L chain (Fig 3).

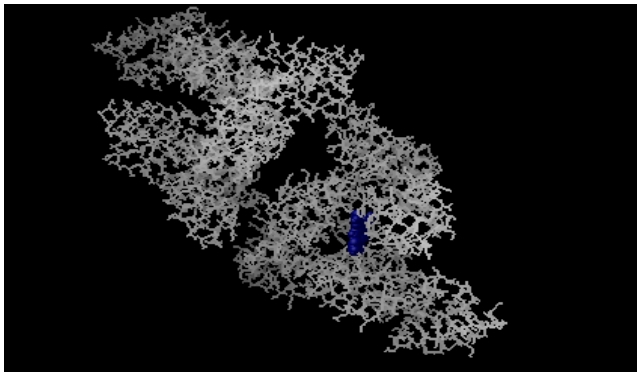

Fig. 3: Cinnamonpolyphenol docked with human serum protein

The table below shows the summary of the docking calculations (Table I). The negative binding energy shows that the docking was performed with less energy hence its stable.

Table 1: Result of Autodock

S. No.	Parameters	Energy (kcal/mol)
1	Estimated Free Energy of Binding	-3.60
2	Estimated Inhibition Constant, Ki	2.29 mM (T= 298.15 K)
3	Final Intermolecular Energy	-8.08
	vdw + Hbond + desolv Energy	-7.80
	Electrostatic energy	-0.28
4	Final Total Internal Energy	-4.63
5	Torsional Free Energy	+4.47
6	Unbound Systems' Energy	-4.63

The energy obtained after docking was -3.60 kcal /mol. This shows that cinnamonpoyphenol binds to human serum protein and the docked conformation has low energy and hence stable.

CONCLUSION

The docking energy of -3.60 indicates that the interaction between cinnamonpolyphenol and human serum protein in the bound state is low. This shows stable conformation of cinnamonpolyphenol as well as the existence of interaction between cinnamonpolyphenol and chain L of hsp. It's this interaction which helps in stimulating the Islets of Langerhan cells of the pancreas to produce insulin. Thus the intake of cinnamon extracts in diets of patients with Type 2 diabetes is found to considerably lower the blood glucose level of Type 2 diabetic patients. Hence the inclusion of cinnamon in the diet of people with type 2 diabetes will reduce risk factors associated with diabetes.

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REFERENCES

1. Cao H, Urban JF and Anderson RA (2008). Cinnamon Polyphenol Extract Affects Immune Responses by Regulating Anti- and Proinflammatory and Glucose Transporter Gene Expression in Mouse Macrophages. *The Journal of Nutrition* , **13**(5), 833-840.
2. Cao, H, Qin B, Panickar KS and Anderson RA (2008). Tea and cinnamon polyphenols improve the metabolic syndrome, *Polyphenols,* **9**(6), 14-17.
3. Khan A, Safdar, M., Muzaffar ,M., Khan, A., Khattak, KN and Anderson, RA (2003). Cinnamon Improves Glucose and Lipids of People with Type 2 Diabetes, *Diabetes Care*, **26**(12), 3215-3218.
4. Qin B, Panickar KS and Anderson RA (2010). Cinnamon: Potential Role in the Prevention of Insulin Resistance, Metabolic Syndrome and Type 2 Diabetes, *Journal of Diabetes Science and Technology* , **4**(3), 685-693.
5. Cao H and Anderson RA (2011).Cinnamon polyphenol extract regulates tristetraprolin and related gene expression in mouse adipocytes, *Journal of Agricultural and food chemistry,* **59**(6), 2739-44.
6. Type 2 diabetes: Practical Targets and Treatments (1-58).
7. Lim EL, Hollingsworth KG, Aribisala BS, Chen MJ, Mathers JC and Taylor R (2011). Reversal of type 2 diabetes: normalisation of beta cell function in association with decreased pancreas and liver triacylglycerol. *Diabetologia*, **54**(10) , 2506-14**.**
8. Parvathy NG, Prathap M, Mukesh M and Thomas L (2013). Design, synthesis and molecular docking studies of benzothiazole derivatives as anti microbial agents. *International journal of pharmacy and pharmaceutical sciences***, 5**(2), 101-106.
9. Shajan AB and Sharmila JS (2013). Action of glycotope vaccines on cancer cell lines molecular modeling and simulation studies.*International journal of pharmacy and pharmaceutical sciences***, 5**(2),141-150.