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Insight into *Jasminum sambac* Molecular Docking Interaction with Glucokinase Related to Diabetes Mellitus

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Diabetes mellitus (DM) is of noncommunicable disease with high prevalence in Indonesia. The study explores the potential of *Jasminum sambac* phytochemical constituent for treating DM. The potential of *Jasminum sambac* as a DM therapy candidate was demonstrated through in silico analysis using several databases and computer-aided drug discovery tools. The present study utilized Pubchem data to obtain the bioactive compounds analyzed while the receptors utilized were obtained from RSCB (PDB ID: 4LC9). The adme properties of the compounds were tested using SwissAdme. Additionally, Swiss target prediction and DB string were employed to respectively analyze target proteins and metabolic pathways, biological activities, and related diseases. Further analysis was carried out through molecular docking utilizing PyRx version 0.8, with visualization being done using BIOVIA Discovery Studio Visualizer version 4.5. From the search results for the compounds contained in *Jasminum sambac* was found that there were several active compounds contained in it. Some of these compounds passed the ADME criteria, compounds (Z, Z,Z)-3,6,9-Dodecatrien -1-ol,(Z)-Jasmone, linalool, Nerolidol, (-)-alpha-Cadinol, Benzenemethanol, Benzaldehyde, Linalyl benzoate, and 2,2,3,4-Tetramethylpentane. Moreover, an in-depth analysis was carried out regarding the molecular interaction that occur, how these compounds bind to the Glucokinase enzymes found in humans, and how their potential is to become an inhibitor of diabetes mellitus. Compounds found in the plant *Jasminum sambac*, specifically Linalyl Benzoate and Benzenemethanol, have been discovered to possess strong bonding capabilities with the Glucokinase enzyme protein. This raises the possibility of developing new medicinal compounds to inhibit diabetes mellitus.

Keywords: *Jasminum sambac* | Diabetes mellitus | GCK | linalyl benzoate | in silico

The disease known as diabetes mellitus (DM) is characterized by blood sugar (blood glucose) levels that are higher than normal, especially when fasting blood sugar levels are above or equal to 126 mg/dl and blood sugar levels are equal to or more than 200 mg/dl. This disease now affects a large number of young people as a result of today's children's unregulated lifestyle. This condition is also induced by several environmental variables, with many people developing diabetes mellitus due to their living environment. In addition to other variables, the diabetics' generation is more likely to develop diabetes mellitus[1]

Diabetes mellitus is a heterogeneous group of diseases with high blood glucose levels. The current classification of diabetes mellitus is presented, and the main features of type 1 and type 2 diabetes are compared. Additionally, accurate biochemical diagnostic criteria and haemoglobin A1c (HbA1c) use in fasting and oral glucose tolerance tests are summarized. Due to the increasing prevalence of diabetes[2], targeted screening to detect diabetes and prediabetes in risk groups is necessary. This is the basis for initiating early steps to prevent the development of diabetes and slow the progression of diabetes in this risk group[3]

To date, the primary mode of treatment for diabetes mellitus has been through the administration of a number of drugs commonly referred to as anti-diabetics. Specifically, these include metformin and sulfonylureas. These drugs have side effects, especially on the kidneys, because if used for too long, they will affect the kidneys and can even cause hepatitis if these drugs are not taken with due observance of the rules given by the doctor[4]. In previous research, we have known the potential of mangosteen peel extract and noni fruit to treat diabetes mellitus, but this has not proven effective when viewed from the effects provided by the two plants, considering that diabetes mellitus is a disease that is difficult to treat[3].

Based on the findings of earlier studies that showed *Jasminum sambac* can be beneficial for coronary heart disease, antibacterial, antioxidant, and anti-aging[56] . *Jasminum sambac* is frequently related to herbal beverages that work well to keep the body resistant. This silico-based research can explain the molecular and cellular mechanisms that occur when the active compounds contained in these plants are induced.

The *Jasminum sambac* plant is widely known by the public because it is often made for aromatherapy, but people do not understand what the benefits of white jasmine are, especially when it is associated with dangerous diseases such as diabetes mellitus, type-2 diabetes, necrosis, edema, and other dangerous diseases[7] This plant is generally used only as an aromatic ingredient such as air freshener or aromatherapy, and several researches discuss anti-inflammatory, antioxidant, antiaging, and antibacterial effects. At the same time, some discuss its relation to cardiovascular disease[5].

Research on the *Jasminum sambac* plant has never referred to diabetes mellitus, where this disease is a disease for which sufferers must take medication throughout their lives. This study aims to predict the potential compounds found in *Jasminum sambac* as a drug to DM. While there is also a discussion about its relation to cardiovascular disease.

The studies conducted on *Jasminum sambac* have not previously explored its potential effect on diabetes mellitus. The present study discovered that while *Jasminum sambac* has been found to be an effective drug for pregnancy, it has not been explored as a means of treatment for diabetes that would otherwise require lifelong medication. Therefore, this study aims to examine the potential of *Jasminum sambac* in treating and even reversing diabetes. Additionally, the connection between *Jasminum sambac* and cardiovascular diseases is also investigated.

Diabetes mellitus is a chronic disease that requires long-term medication[8] and yet studies on *Jasminum sambac* have not addressed this condition. Hence, this study explores the possibility of reducing and treating diabetes mellitus using the *Jasminum*

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sambac plant. GCK is the main regulatory enzyme in pancreatic beta cells. It plays an important role in regulating insulin secretion and has been called a sensory pancreatic beta cell.

Given its primary role in regulating insulin release, it is understood that mutations in the GCK gene can lead to hyperglycemia and hypoglycemia. And this is one of the causes of Diabetes Mellitus (DM)[8]. Previously there was also research on how protein GCK could play an important role in curing diabetes in pregnant women. However, it was considered inefficient because it still had to be conditioned by lifestyle and insulin.GCK-MODY (Maturity-Onset Diabetes of the Young) is a quasi-experimental human model that allowed us to determine the respective roles of maternal and fetal hyperglycemia genotypes on fetal growth and to confirm the central role of fetal insulin secretion in fetal growth. Non-invasive fetal genotyping is a major advance in the treatment of GCK-MODY women, as it will enable the determination of women whose diabetes should be treated during pregnancy[9].

However, the current study focuses on pure GCK directly confronted with diabetes mellitus without assistance from other factors supporting the treatment. GCK is an enzyme crucial for the initial phase of the consumption of glucose by the beta-cell and the liver at physiologically relevant glucose concentrations. However, glucokinase can only function when glucose levels are abundant due to its high Km for glucose. Its primary role is to supply glucose-6-phosphate (G6P) for glycogen synthesis. In the pancreas, glucokinase controls insulin secretion and acts as an insulin-sensitive indicator of hepatic glucose utilization, thus facilitating glucose uptake and conversion. Hence, GCK is pivotal to diabetes mellitus[10]. Many disease-causing mutations in the GCK gene have been identified[11] Through a series of trials, using the in silico method, this analysis refers to testing the protein candidate drug bound to compounds that will be made as drugs where the drug will directly lead to diabetes mellitus.

Materials

Materials for this study were obtained from the database with details as below

- Eight active compounds from *Jasminum sambac* will be analyzed in this study, including (Z,Z,Z)-3,6,9-Dodecatrien-1-ol (CID 5281129), (Z)-Jasmone (CID 1549018), linalool (CID 6549), Nerolidol (CID 5284507), (-)-alpha-Cadinol (CID 10398656), Benzenemethanol (CID 244), Benzaldehyde (CID 240), Linalyl benzoate (CID 31353), 2,2,3,4 -Tetramethylpentane (CID 14462)
- Protein used as a drug candidate namely GCK protein (PDB ID 4LC9)

Place and time of research

This in silico research uses several web-based databases and applications related to computer-aided drug discovery. Plant compound data was obtained by accessing dr duke (https://phytochem.nal.usda.gov) and PubChem (https://pubchem.ncbi.nlm.nih.gov). The ADME data of each compound obtained were analyzed with Swissadme (http://www.swissadme.ch/index.php), protein targets were analyzed with Swisstarget (http://www.swisstargetprediction.ch/), and compound docking using the PyRx application version 8 and its visualization with Discovery Studio.

Method

Data anchoring of chemical compounds

The compound content of the *Jasminum sambac* plant via http://www.knapsackfamily.com/ then proceeded to search for the canonical SMILE of these compounds in pubchem,, Analysis of Absorption Distribution of Metabolism and Excretion (ADME) was performed by inputting canonical smiles into the web server http://www.swissadme.ch/ The analysis is carried out to select the suitable compound for inclusion as a drug candidate.

Target Protein Docking

The compound has successfully escaped from Swiss target prediction link to analyze the existing target protein. The protein that can be included as a drug candidate protein may exceed 0, and DM target proteins were tested through a string DB. The study employed a computational approach utilizing protein data bank (PDB) data obtained from rscb.pdb, and analyzed several test ligands downloaded from the Pubchem site, including (Z,Z,Z)-3,6,9-Dodecatrien-1-ol, (Z)-Jasmone, linalool, Nerolidol, (-)-alpha-Cadinol, Benzenemethanol, Benzaldehyde, Linalyl benzoate, and 2,2,3,4-Tetramethylpentane. The researchers utilized molecular docking, a computational method that involves software interactions between different components and is used in designing new drugs. The study employed software such as Autodock Vina, Autodock Tools, and Discovery Studio to prepare the protein and ligand and analyze the results of the amino acids bound to the compounds. This approach provides a cost-effective and time-efficient way of assessing different components and avoiding potentially interfering molecules to facilitate the success of the docking process.

To begin, the proteins and ligands must be prepared. The GCK protein, known for its complex structure containing water molecules and natural ligands, requires the removal of water molecules during preparation to prevent interference with the docking process. Once the proteins and ligands have been prepared, cells are added using Pyrex application to facilitate optimal docking results. Following the docking process, the binding of amino acids to the protein is assessed to determine if a perfect binding has occurred with the compound.

Results And Discussion

Human glucose metabolism is tightly regulated by glucokinase (GCK) activity. GCK is produced primarily in the pancreas, which catalyzes the rate-limiting step in insulin secretion, and in the liver, which is involved in glycogen synthesis[11]. Various disease-causing mutations within the GCK gene have been identified. Activating mutations manifest clinically as congenital hyperinsulinism, whereas loss-of-function mutations cause several diabetic conditions[10]. Pharmaceutical interest in GCK-related diabetes therapies is high. GCK is crucial in glucose homeostasis and is regulated at multiple levels. It can self-regulate through conformational dynamics, interacts with other proteins, and undergoes post-translational modifications. While progress has been made in understanding these regulatory mechanisms, their integration and coordination within cells are still being investigated. This study aims to summarize findings and provide insight into the molecular and cellular control of GCK.

The results of an analysis of network proteins related to diabetes mellitus using string-db (Figure 1) suggest that seven proteins are labelled red, among them the GCK enzyme protein was chosen to be the receptor. Specifically, GCK is better known as the Glucokinase enzyme that plays a key role in blood sugar regulation in the body. It interacts with several other enzymes to create bonds such as the bond between GCK and GCGR, which binds directly to Glucogen in the body and is related to the receptor of GCK. Another bond is between GCK and PPARG, where PPARG itself is a Gamma receptor that is activated by peroxisome proliferators - nuclear receptors that bind to peroxisome proliferators such as hypolipidemic drugs and fatty acids. Once activated by the ligand, Nuclear receptors bind to DNA-specific PPAR response elements (PPRE) and modulate the transcription of their target genes, such as acyl-CoA oxidases. This controls the peroxisome beta-oxidation pathway of fatty acids, which is a key regulator of adipocyte differentiation and glucose homeostasis.

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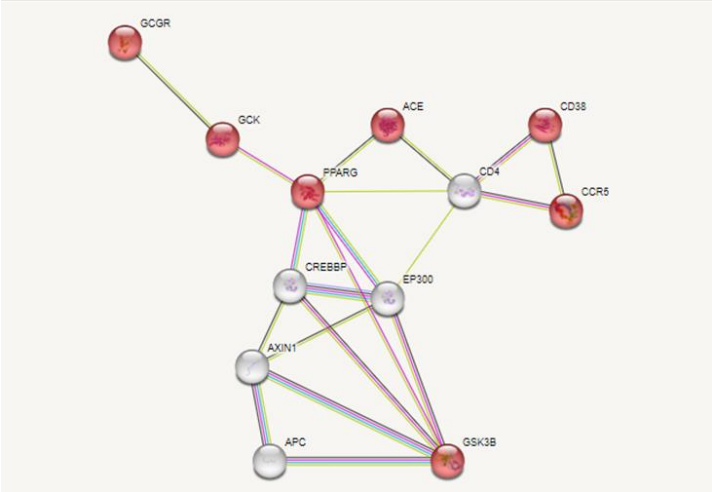

Figure 1 Network protein related to diabetes mellitus results of analysis using string-db

The pharmacological basis of the medical use of *Jasminum sambac* in cardiovascular disease and ex-amine the core mechanisms. A mechanistic investigation demonstrated that ex-vivo *Jasminum sambac* crude leaf extract induced vasorelaxant effects in endothelium-intact aortic ring preparations via pressure and force transducers coupled to the Power Lab Data Acquisition System. Antihypertensive effects were found to be recorded in Further; *Jasminum sambac* showed a cardioprotective effect against adrenaline-induced left ventricular hypertrophy in rabbits observed hemodynamically. CK-MB, LDH, troponin, CRP, ALT, AST, and ALP levels were lower in myocardial infarction models compared to controls, as were necrosis, edema, and inflammatory cell recruitment[12].

Diabetes is a complex disease. Our understanding of the mechanisms at the molecular level is advancing. These discoveries should lead to better therapeutic approaches. Diabetes mellitus is a syndrome with many associated subphenotypes. These include mitochondrial diseases, lipodystrophy, and cytokine-mediated inflammatory diseases. Levels of sphingosine-1-phosphate, recently shown to play a role in glucose homeostasis, are low, and ceramide levels are elevated in diabetic patients. The main phenotypes associated with diabetes mellitus are dyslipidemia, especially hypertriglyceridemia, and low high-density lipoprotein cholesterol levels. Both diabetes and dyslipidemia are strongly associated with an increased risk of atherosclerotic vascular disease[12].

Molecular docking is a well-known in silico, structure-based technique extensively used in drug development. Docking enables the discovery of new therapeutic compounds, anticipation of ligand-target interactions at the molecular level, and determination of structure-activity correlations (SARs), even without prior knowledge of the chemical makeup of other target modulators. While docking was initially created to study the molecular processes that regulate recognition between small and large molecules, its application in drug development has undergone significant modifications in recent years. In this study, we describe the original use of molecular docking to support tasks related to drug development[13].

The compounds from *Jasminum sambac* are used for research on diabetes mellitus because the protein to be used in this test includes glucko or terms related to sugar in the blood. And this is comparable to the use of the GCK protein, which catalyzes the first step of glucose utilization by beta cells and the liver at physiological glucose concentrations. Because glucokinase has a high molecular constant for glucose, it is only effective when glucose is abundant. The role of GCK is to provide its G6P for glycogen synthesis. Pancreatic glucokinase plays an important role in the regulation of insulin secretion. Hepatic glucokinase helps facilitate glucose uptake and conversion by acting as an insulin-sensitive determinant of hepatic glucose utilization.

Previous studies found that when ligands like cinnamaldehyde, beta-caryophyllene, and eugenol were supported by acarbose, the affinity ranged from -5.5 kcal/mol to -6.3 kcal/mol, but several docking compounds were supported by antidiabetic drugs like acarbose and prigliatin [14]. whereas in this study, a pure ligand was directly docked with the Glucokinase enzyme protein and obtained an affinity of -5.8 kcal/mol, explaining that linalyl benzoate as a ligand can provide sufficient affinity great candidate for antidiabetic drugs without combining the docking compound with the help of antidiabetic drugs.

After analyzing the results in Table 1, it was found that the nine compounds tested show an affinity range of -5 to -5.8 kcal/mol. Although some of these numbers could potentially be considered as drug candidates for diabetes mellitus, the minimum difference between the numbers obtained was only 0.6. Therefore, further laboratory testing is required to predict if GCK could be developed into an anti-diabetic drug. Apart from evaluating the activity of the compounds, SwissADME is a useful tool for categorizing the compounds based on their ADME properties, which is essential in identifying promising drug candidates. In order to be effective, a potent molecule must reach its target in the body in sufficient concentrations and remain biologically active long enough for the desired effect to occur. Therefore, ADME studies are conducted early in the drug development process. As access to physical samples may be limited, computer models are being increasingly utilized as an alternative to experimental studies to examine the properties of various compounds. SwissADME is an online tool that provides computational chemists with access to an array of fast and reliable predictive models for pharmacokinetics, drug-likeness, and medicinal chemistry friendliness, including the BOILED-Egg, iLOGP, and Bioavailability Radar. With a user-friendly interface, it is easily accessible at http://www.swissadme.ch and does not require specialists to accurately anticipate essential variables in molecular collections. These models can serve as a valuable alternative to experimental studies, enabling researchers to make informed decisions during drug development and assess the ADME properties of compounds more efficiently.

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Table1 Table of the results of the visualization analysis regarding the amino acid bonds where the ligand binds to the receptor

Ligands	Affinity Bindings (Kcal/mo)	Interactin(Bond)	Residue
(Z,Z,Z)-3,6,9-Dodecatrien-1-ol	-5.5	Van Der Waals	HIS A:331; ILEA:365; THR A:394; SER A:395; ILE A:396; LEU A:397; PHE A:408; VAL A:426
		Alkyl	VAL A:333; LEU A:400; VAL A :406; LEU A:422
		Pi-alkyl	VAL A:333; PHE A:363; LEU A:422.
		Alkyl	LEU A:412; VAL A:437; LEU A:445
		Conventional Hydrogen Bonds	SER A: 439
linalool	-5,3	Van Der Waals	LEU A:364; THR A:394; LEU A:397; VAL A:406; PHE A:408
		Alkyl	
		Pi-alkyl	HIS A:331; VAL A:333; PHE A:363; ILE A:396
			VAL A:333; PHE A:363; ILEA:365; ILE A:396; LEU A:400; LEU A:422
Nerolidol	-5.8	-	-
(-)-alpha-Cadinol	-5.2	Van Der Waals	SER A:439; VAL A:441; GLY A:442; GLN A:443; SER A:444;LYS A:450; GLU B:51; LYS B:56
		Alkyl	HIS B:50; LEU B:58
		Pi-alkyl	LEU A:445; LEU B:58
		Conventional Hydrogen Bonds	SER A:458; THR A: 460
Benzeneemethanol	-5,3	Van Der Waals	HIS A:331; SER A:395; PRO A:398: VAL A:406; LEU A:422;
		Pi-alkyl	VAL A:333; LEU A:400
		Conventional Hydrogen Bonds	THR A:394; LEU A:397
		Pi-Sigma	ILE A:396
		Pi-Pi T-shaped	PHE A:363
Benzaldehyde	-5.5	Van Der Waals	HIS A:331; SER A:395; PRO A:398: VAL A:406; LEU A:422;
		Pi-alkyl	VAL A:333; LEU A:400
		Conventional Hydrogen Bonds	THR A:394; LEU A:397
		Pi-Sigma	ILE A:396
		Pi-Pi T-shaped	PHE A:363
Linalyl benzoate	-5.8	Van Der Waals	GLM A:336; THR A:337;ASP A:413; ASP A:414; THR A:440; GLN A:443; THR A:471; GLN A:474; GLU A:479
		Alkyl	LYS A:475
		Pi-alkyl	LEU A:338; LYS A:475; ARG A:478
		Conventional Hydrogen Bonds	THR A:411; ARG A:478
2,2,3,4-Tetramethylpentane	-5	Van Der Waals	HIS A:331; ILEA:365; THR A:394; SER A:395; LEU A:397; LEU A:400
		Alkyl	VAL A:333; ILE A:396; LEU A:422
		Pi-alkyl	VAL A:333; PHE A:363; ILE A:396
		Pi-Sigma	PHE A:363

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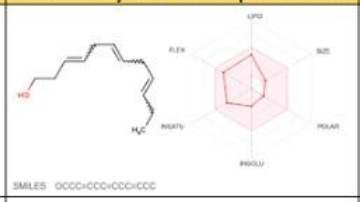
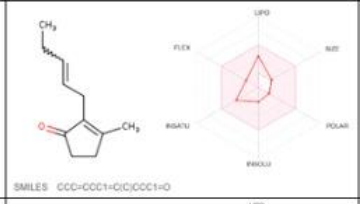
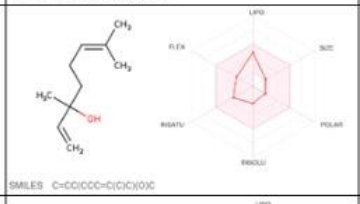
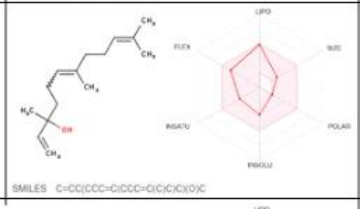
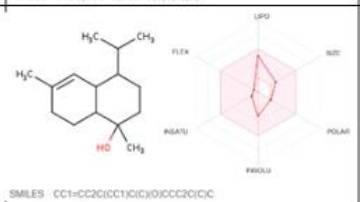
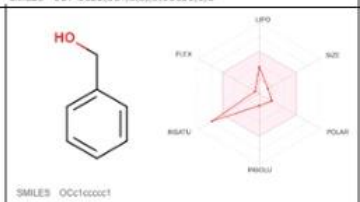
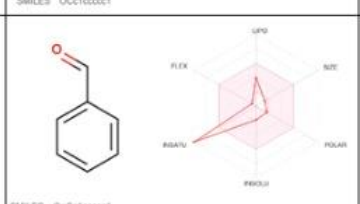
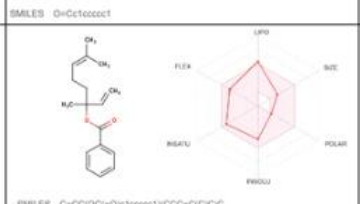
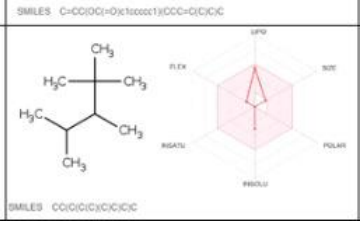
Table 2 Properties of Compound Based on SwissAdme Web Server

Metabolit	Bioavailability Radar and compund structure	PUBCHEM CID	MW	LD50	HIA	BBB	TPSA
(Z,Z,Z)-3,6,9-Dodecatrien-1-ol		5281129	180.29	1,3605	0.9958	0.9425	20.23
(Z)-Jasmone		1549018	164.24	1,7855	1.000	0.9683	17.07
linalool		6549	154.25	1,774	0.9741	0.9699	20.23
Nerolidol		5284507	222.37	1,6795	0.9792	0.9559	20.23
(-)-alpha-Cadinol		10398656	222.37	2,2009	1.000	0.9455	20.23
Benzenemethanol		244	108.14	1,9753	0.9906	0.9698	20.23
Benzaldehyde		240	106.12	19433	0.9958	0.9804	17.07
Linalyl benzoate		31353	258.36	1,6765	0.9893	0.9567	26.30
2,2,3,4-Tetramethylpentane		14462	128.26	1,5332	0.9870	0.9817	0.00

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The use of SwissADME also identified nine specific compounds from Jasminum sambac (Table 2) that fall under the ADME category, namely (Z,Z,Z)-3, 6, 9-Dodecatrien-1-ol, (Z)-Jasmone, linalool, Nerolidol, (-)-alpha-Cadinol, Benzenemethanol, Benzaldehyde, Linalyl benzoate, and 2,2,3,4. These compounds were selected for further examination for their potential to bind to a protein of interest in this study. Based on the docking results, it is evident that the interaction between the nine chemicals tested and GCK requires a docking study. The data reveals that all proteins and ligands had binding affinity values, as shown in Table 1. However, Linalyl benzoate was identified as a promising ligand with a bond number of -5.8 due to its Van der Waals, alkyl, Pi-Alkyl, and Conventional Hydrogen Bonds. Additionally, amino acid residues contain different amino acids that include ARG A 478 and LYS A: 475, which have the potential to act as competitive inhibitors under certain conditions.

Conclusion

In conclusion, Linalyl Benzoate found in Jasminum sambac has promising potential as a diabetes mellitus inhibitor through its binding to the GCK protein, which affects blood sugar. Jasminum sambac has been explored for its therapeutic uses in different fields, such as cardiovascular disorders, gingivitis treatment, antimicrobial activities, and anti-obesity effects. Furthermore, Jasminum sambac is rich in volatile compounds, including S-(+)-linalool and benzyl acetate, contributing to its distinct aroma and potential pharmacological activity. These findings support the importance of exploring the diverse therapeutic properties of Jasminum sambac as a natural source of medication.

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Supplementary materials

Figure S1 the results of the docking analysis of protein compounds and ligands carried out in the Discovery Studio application and obtained residues amino acid

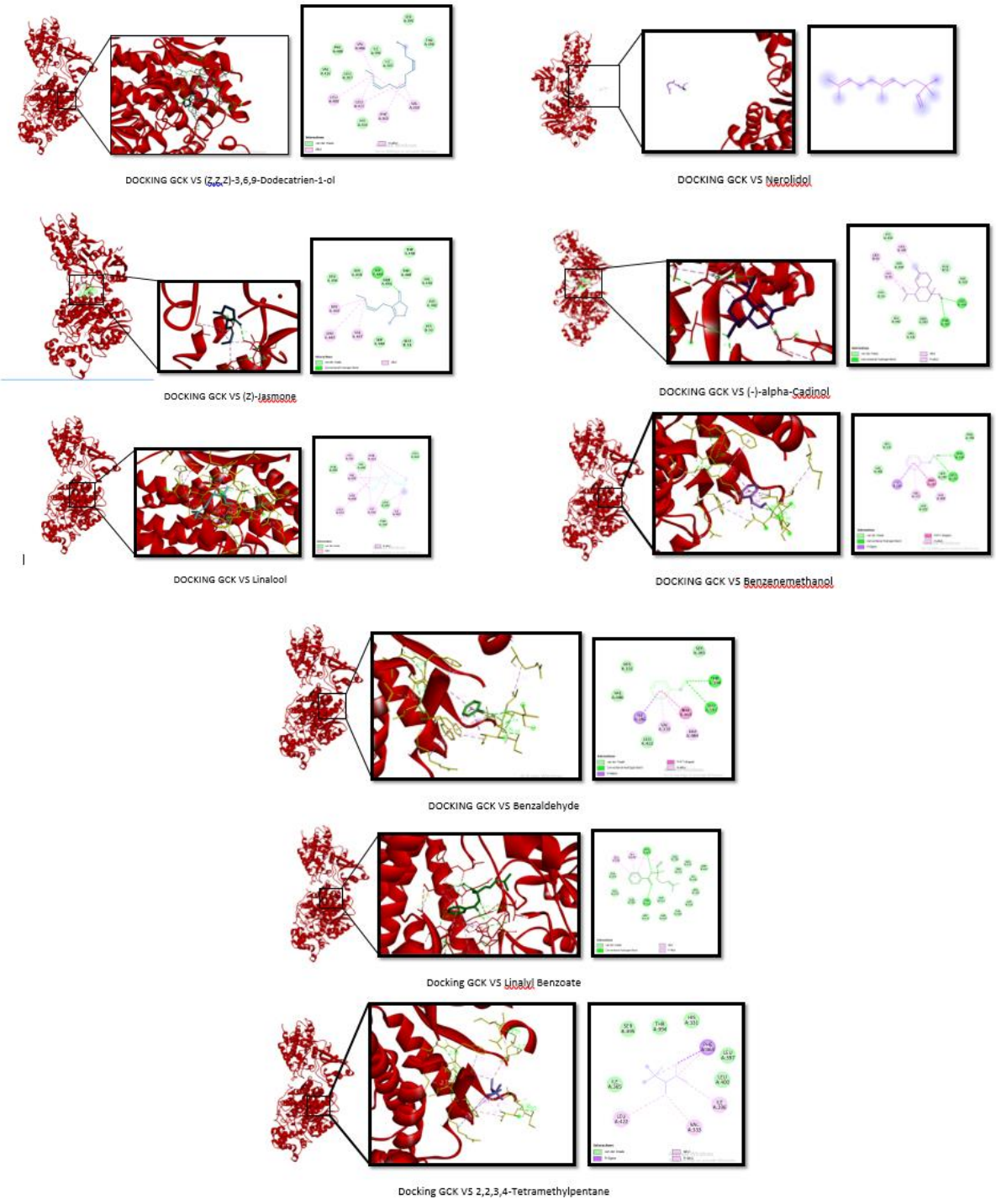

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Table S1 Database compound from SwissADME

Metabolite	PUBCHEM CID	MW	LD50 mol/kg	HIA	BBB	TPSA
BETULINIC-ACID	64971	456.7	3.8916	0.9952	0.7713	57.53
(Z,Z,Z)-3,6,9-Dodecatrien-1-ol	5281129	180.29	1.3605	0.9958	0.9425	20.23
(Z)-Jasmone	1549018	164.24	1.7855	1,000	0.9683	17.07
linalool	6549	154.25	1.774	0.9741	0.9699	20.23
E-beta-farnesene	15228937	206.37	1.4955	0.9899	0.9357	0
Nerolidol	5284507	222.37	1.6795	0.9792	0.9559	20.23
(+)-8-Hydroxypinoresinol	3010930	374.38	2.732	0.9923	0.5937	97.61
Oleoside	101042548	390.34	1.9361	0.6846	0.7248	183.21
(-)-alpha-Cadinol	10398656	222.37	2.2009	1,000	0.9455	20.23
Benzenemethanol	244	108.14	1.9753	0.9906	0.9698	20.23
Benzaldehyde	240	106.12	19433	0.9958	0.9804	17.07
Oleoside 11-methyl ester	10692563	404.37	2.2214	0.8387	0.8694	172.21
Linalyl benzoate	31353	258.36	1.6765	0.9893	0.9567	26.3
3-Methylcyclopentene	14263	82.14	1.6523	0.9966	0.9911	0
Sambacolignoside	13995443	922.88	4.1452	0.6611	0.8815	317.74
Phenethyl primeveroside	131129	416.42	1.7674	0.8784	0.5387	158.3
Sambacin	131752486	540.56	3.3561	0.6723	0.5297	181.44
2,2,3,4-Tetramethylpentane	14462	128.26	1.5332	0.987	0.9817	0

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Table S2 Knapsnack Data

CID	CAS ID	Metabolite	Molecular formula	Mw	Organism or InChIKey etc.
C00001249	81345-02-0	(Z,Z,Z)-3,6,9-Dodecatrien-1-ol	C12H20O	18,015,141,526	Jasminum sambac
C00001313	488-10-8	(Z)-Jasmone	C11H16O	16,412,011,513	Jasminum sambac
C00003047	78-70-6	linalool	C10H18O	1,541,357,652	Jasminum sambac
C00003131	18794-84-8	E-beta-farnesene	C15H24	20,418,780,077	Jasminum sambac
C00003166	142-50-7	Nerolidol	C15H26O	22,219,836,545	Jasminum sambac
C00007191	81426-17-7	(+)-8-Hydroxypinoresinol	C20H22O7	37,413,655,306	Jasminum sambac
C00010784	178600-68-5	Oleoside	C16H22O11	39,011,621,155	Jasminum sambac (L.) Ait.
C00020065	481-34-5	(-)-alpha-Cadinol	C15H26O	22,219,836,545	Jasminum sambac
C00029811	100-51-6	Benzenemethanol	C7H8O	10,805,751,488	Jasminum sambac
C00034452	100-52-7	Benzaldehyde	C7H6O	10,604,186,481	Jasminum sambac
C00037580	60539-23-3	Oleoside 11-methyl ester	C17H24O11	40,413,186,161	Jasminum sambac
C00051281	126-64-7	Linalyl benzoate	C17H22O2	25,816,197,995	Jasminum sambac
C00056472	1120-62-3	3-Methylcyclopentene	C6H10	8,207,825,032	Jasminum sambac
C00056875	114449-12-6	Sambacolignoside	C43H54O22	92,231,067,341	Jasminum sambac
C00057008	129932-48-5	Phenethyl primeveroside	C19H28O10	41,616,824,712	Jasminum sambac
C00057604	85562-86-3	Sambacin	C26H36O12	54,022,067,662	Jasminum sambac
C00057803	1186-53-4	2,2,3,4-Tetramethylpentane	C9H20	12,815,650,064	Jasminum sambac

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