October – December, 2025
Original Article
DOI: http://dx.doi.org/10.30867/action.v10i4.2931

AcTion: Aceh Nutrition Journal
Pages: 1007 – 1021 | p-issn 2527-3310; e-issn 2548-5741

Phytochemical evaluation and antidiabetic potential (In silico) of corn silk (*Zea mays L.*) and jasmine (*Jasminum sambac*)

Evaluasi fitokimia dan potensi antidiabetik (In silico) dari rambut jagung (Zea mays L.) dan melati (Jasminum sambac)

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Article History:
Received: October 15, 2025; Revised: November 03, 2025; Accepted: November 12, 2025; Published: December 14, 2025.

Publisher:
Politeknik Kesehatan Aceh
Kementerian Kesehatan RI

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Abstract

Diabetes mellitus is a significant global health challenge, necessitating the exploration of novel therapeutics from natural sources for its treatment. This study aimed to identify the bioactive compounds in a combinatorial methanolic extract of corn silk (*Zea mays L.*) and jasmine flowers *(Jasminum sambac*) and predict their antidiabetic potential. The extract was analyzed using Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS). The identified compounds were evaluated in silico via molecular docking simulations against key antidiabetic protein targets: Glucagon-Like Peptide 1 (GLP-1), Insulin-like Growth Factor 1 (IGF-1), Glucose Transporter 4 (GLUT4), alpha-glucosidase, and superoxide dismutase (SOD). The analysis focused on the binding energy (ΔG). A total of 44 metabolites were identified in this study. Molecular docking results indicated that rothindin exhibited the highest binding affinity for GLUT4, with a binding energy of -9.9 kcal/mol. Rothindin and Chlorogenic Acid also showed significant potential as modulators of GLUT4 and α-glucosidase, respectively. In conclusion, the combined extract contains bioactive compounds, particularly roxindin and chlorogenic acid, which demonstrate significant in silico potential as antidiabetic agents.

Keywords: Antidiabetic, corn silk, jasmine flower, in silico, molecular docking

Abstrak

Diabetes melitus merupakan tantangan kesehatan global yang signifikan, sehingga mendorong eksplorasi terapi baru dari sumber alami. Penelitian ini bertujuan untuk mengidentifikasi senyawa bioaktif dalam ekstrak metanol kombinasi rambut jagung (*Zea mays L.*) dan bunga melati (*Jasminum sambac*) serta memprediksi potensi antidiabetiknya. Ekstrak dianalisis menggunakan Kromatografi Cair-Spektrometri Massa Tandem (LC-MS/MS). Senyawa yang teridentifikasi dievaluasi secara in silico melalui simulasi docking molekuler terhadap target protein antidiabetes utama: Glucagon-Like Peptide 1 (GLP-1), Insulin-like Growth Factor 1 (IGF-1), Glucose Transporter 4 (GLUT4), alfa-glukosidase, dan superoksida dismutase (SOD). Analisis berfokus pada energi ikatan (ΔG). Sebanyak 44 metabolit teridentifikasi. Hasil docking molekuler menunjukkan bahwa rothindin memiliki afinitas ikatan tertinggi pada target GLUT4, dengan energi ikatan -9,9 kkal/mol. Rothindin dan Asam Klorogenat juga menunjukkan potensi signifikan sebagai modulator pada target GLUT4 dan α-glukosidase. Kesimpulan, ekstrak gabungan ini mengandung senyawa bioaktif, khususnya Rothindin dan Asam Klorogenat, yang menunjukkan potensi in silico signifikan sebagai agen antidiabetes.

Kata Kunci: Antidiabetes, rambut jagung, bunga melati, in silico, docking molekuler

Introduction

Diabetes mellitus (DM), a chronic metabolic disorder, is a major global health challenge owing to its increasing prevalence (Hossain et al., 2024). It is characterized by impaired blood glucose regulation resulting from insulin resistance, defective insulin secretion, or a combination of both (Antar et al., 2023). The prevalence of DM in Indonesia, based on blood examinations according to the DM criteria from the PERKENI (Indonesian Endocrinology Association) consensus of 2011 and 2015, has increased significantly. The prevalence of DM in the population aged ≥ 15 years increased from 6.9% in 2013 to 8.5% in 2018 (Kemenkes Republik Indonesia, 2019). DM treatment involves oral antidiabetic (OAD) drugs and insulin; however, the majority of patients are inadequately treated. The proportion of diabetes mellitus control efforts in the population diagnosed with DM by doctors was 80.2% with dietary management, 48.1% with exercise, and 35.7% with herbal alternatives (Kemenkes Republik Indonesia 2019). Therefore, there is an urgent need for novel therapeutic options, including natural compounds with potential pharmacological effects (Bhatti et al., 2022). Corn silk (*Zea mays L.*), traditionally considered agricultural waste, is a natural material containing biologically active compounds, such as flavonoids, which have shown potential antidiabetic properties in various studies (Khushe et al., 2024; Nawaz et al., 2018; Raihan et al., 2023; Wang & Zhao, 2019).

Although corn silk has been widely studied for its flavonoid content, jasmine flowers (*Jasminum sambac*) are known for their aromatic properties (Zhang et al., 2022). However, they may also been hypothesized to contain bioactive compounds. Prior *in silico* research on the antidiabetic potential of corn silk (Chaudhary et al., 2022) has indicated high binding affinities for compounds such as flavones (against PTPN1B), β-carotene (against GLUT1), gallotannins (against DPP4), 3-O-caffeoylquinic acid (against α-glucosidase), and stigmasterol (against α-amylase). However, research gaps remain as the current literature tends to report single extracts separately; thus, the potential synergistic benefits of two or more extracts may differ (Caesar & Cech, 2019). The added value of combining these extracts lies in their potential for synergistic or additive interactions, wherein compounds from jasmine (e.g., antioxidants or anti-inflammatory agents) can enhance the metabolic effects of corn silk flavonoids. Practically, this could result in a multi-target formulation that has the potential to address the complex pathophysiology of diabetes compared to single-herb treatments. Furthermore, the mechanism of action focuses on how bioactive compounds interact with other key proteins involved in glucose homeostasis, specifically glucagon-like peptide 1 (GLP-1) and insulin-like growth factor 1 (IGF-1) (Jahandideh & Wu, 2022), and glucose transporter 4 (GLUT4) (Wang et al., 2020), alpha-glucosidase (U. Hossain et al., 220), and superoxide dismutase (SOD) (Bouyahya et al., 2024). However, the combination of corn silk and jasmine flowers remains unknown.

The target proteins of the bioactive compounds in the combined corn silk and jasmine flower extracts were selected based on their pivotal roles in diabetes. These include GLP-1, which is essential for insulin secretion and glucose homeostasis (Abiola et al., 2024); IGF-1, a hormone structurally similar to insulin that can bind to insulin receptors and mimic insulin's metabolic effects, although with lower affinity (Nurmamulyosari et al., 2015); GLUT4, the primary insulin-regulated glucose transporter, which plays a vital role in glucose metabolism in insulin-sensitive tissues such as skeletal muscle, cardiac muscle, and adipose tissue; and SOD, a key antioxidant enzyme that serves as a primary defense against oxidative stress induced by chronic hyperglycemia in diabetes (Alhujaily et al., 2022).

To investigate and provide preliminary evidence for the antidiabetic potential of corn silk, we employed an *in silico* approach as an initial screening method. This computational methodology enabled the prediction of interactions and binding affinities between bioactive compounds and diabetes-related target proteins, thus offering crucial insights prior to further experimental validation. The novelty of this study lies in the specific, uninvestigated combination of *Zea mays L.* and *Jasminum sambac* and its evaluation against a diverse panel of five key proteins associated with diabetes. This study is important because it provides a foundational, science-based rationale for developing novel multi-component herbal therapies.

This study aimed to identify the bioactive compounds in a combinatorial extract of corn

silk (*Zea mays L.)* and jasmine flowers (*Jasminum sambac)* and to predict their antidiabetic potential in silico against protein targets associated with diabetes mellitus, namely glucagon-like peptide 1 (GLP-1), insulin-like growth factor 1 (IGF-1), glucose transporter 4 (GLUT4), alpha-glucosidase, and superoxide dismutase (SOD), using a molecular docking approach. This study contributes to the field of nutrition and food by systematically identifying promising key compounds from potential combinations, thus guiding future in vitro and in vivo validations necessary for the development of alternative diabetes therapies based on natural ingredients.

Methods

Preparation of Corn Silk and Jasmine Flower Extracts

Preparation of corn silk and jasmine flower extracts a single batch of Bisma variety corn silk (harvested December 2024, Bogor, Indonesia) and fresh jasmine flowers (*Jasminum sambac*) (Bekasi City) was used. A 3 g homogenized powder composite of the materials was extracted via maceration (24 h, room temperature), followed by a water bath shaker (1.5 h, 60 °C). The solvent used was methanol : water (85:15, v/v) at a 1:4 material-to-solvent ratio (Haslina & Eva, 2017). The resulting solvent was concentrated using a rotary flash evaporator at 60 °C.

Liquid Chromatography Tandem Mass Spectrophotometry (LC-MS/MS) Analysis

The concentrated extract was analyzed at the Forensic Laboratory Center (Puslabfor) of the Indonesian National Police using a UPLC-MS/MS system (QToF analyzer, positive ESI source) following the protocol described by Mutiah et al. (2024). Chromatographic separation was achieved using an Acquity C18 column (1.8 µm; 2.1×150 mm). The mobile phase consisted of a gradient elution system with (A) HPLC-grade water with formic acid (Merck, Darmstadt, Germany) at 99.9/0.1 [v/v] and (B) acetonitrile (Merck) with formic acid at 99.9/0.1 [v/v]. The source and desolvation temperatures were maintained at 100 °C and 350 °C, respectively. For sample preparation, 10 mg of the extract was dissolved in a 10 mL volumetric flask using absolute methanol, and a 5 µL aliquot was injected into the UPLC-MS system for analysis. Analytical parameters were set for the positive ion mode, with mass spectra acquired in the m/z range of 120–1000 Da. MassLynx software version 4.1 (Waters, Massachusetts, USA) and the PubChem database (https://pubchem.ncbi.nlm.nih.gov/) were used for chromatogram processing and compound identification.

Ligand and Receptor Protein Preparation

Secondary metabolite compounds identified by LC-MS/MS analysis of corn silk and jasmine flowers were selected as test ligands. The 3D structures were retrieved from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/). *sdf* format, and subsequently optimized and saved as. *pdb* files. These optimized ligand structures were then prepared using the Phyton Prescription Virtual Screening Tool (PyRx) and saved. pdbqt format.

The selected receptor proteins from *Homo sapiens* included GLP-1 (Protein Data Bank (PDB) ID: 5VEX), IGF-1 (PDB ID: 1K3A), α-glucosidase (PDB ID: 3WY1), GLUT4 (PDB ID: 7WSM), and SOD (PDB ID: 2C9V). These proteins, which are involved in glucose homeostasis, insulin signaling, and oxidative stress, were selected for their established and diverse roles in the pathophysiology of diabetes. The crystal structures were downloaded from the PDB database (www.rscb.org/pdb). Structures with a crystallographic resolution of ≤ 2 Å and a stable 3D conformation were selected.

Molecular Docking Method Validation and Visualization

Method validation was performed to ensure that the docking protocol accurately replicated the known binding poses. The native ligand, separated during receptor preparation, was docked into its respective receptor using the Python Prescription Virtual Screening Tool (PyRx).

Docking validation was performed by re-docking the native ligand within a maximum grid box with the output saved. *pdb* format. Both the test and native ligands were docked to the

receptors using PyMOL software. The grid box size, spacing, and coordinates determined from the validation results were applied to all subsequent molecular docking simulations. The docking results were obtained from. *pdbqt* format, along with a "log.txt" file containing binding energy values, specifically the Gibbs free energy (ΔG).

The binding energies of the test and native ligand-receptor complexes were compared to assess the spontaneity of ligand-receptor interactions. Ligand interactions with the receptors were visualized using PyMOL to evaluate the binding modes. The key in silico outputs from this analysis included the binding affinity (kcal/mol), Root Mean Square Deviation (RMSD), number of hydrogen bond residues, and 2D docking visualization.

Result and Discussion

Chromatogram Analysis & Metabolite Profile of Corn Silk and Jasmine Flower Methanol Extracts

A total of 44 compounds were identified in the combined extracts of corn silk and jasmine flowers using UPLC-QToF-MS/MS (Figure 1 and Table 1). These compounds were categorized as follows: 14 flavonoids and their derivatives, 8 lipids, 6 amino acids/proteins and their derivatives, 4 glycosides (excluding flavonoid glycosides already included in the flavonoid group), 2 coumarins and their derivatives, 2 organic/carboxylic acids, 1 other phenolic compound (curcumin II (monodemethoxyxurxumin)), and 6 compounds from various other classes.

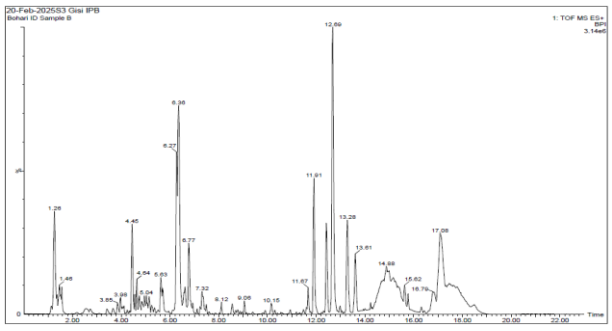


Figure 1. UPLC-QToF MS/MS Chromatogram of combined corn silk and jasmine flower extracts. Each peak in the chromatogram represents an identified compound in the sample

Corn silk and jasmine flowers contain various bioactive compounds, including quercetin, robinin, kaempferol, rutin, coumarin, nobiletin, tangeritin, monodemethoxycurcumin, epicatechin-3-o-gallate, chlorogenic acid, apiin, margaritene, and javanicin d, which exert various pharmacological effects, including reducing blood lipids, lowering blood pressure, regulating blood sugar levels, and exerting anti-inflammatory and antioxidant effects (Shankaranarayana et al., 2024; Y. Wang et al., 2024). In contrast, jasmine flowers, specifically Jasminum sambac, are known for their aromatic terpene compounds, including monoterpenes and sesquiterpenes, which are vital for plant fragrance (Chen et al., 2023). Furthermore, jasmine flowers contain various fragrant compounds, such as benzyl acetate, β-pinene, citronellol, and linalool, which contribute to their intense aroma and potential therapeutic uses (Wu et al., 2021). The integration of these two extracts could potentially create a product with enhanced therapeutic and aromatic properties, leveraging the bioactive components of corn silk and the aromatic terpenes of jasmine flowers.

Blinding Affinity of Bioactive Compounds from Corn Silk and Jasmine Flower with GLP-1, IGF-1, GLUT4, α-glucosidase, and SOD Targets

Fourteen identified bioactive compounds were evaluated using Lipinski's Rule of Five to predict their drug-like properties and potential oral bioavailability. Based on the data in Table 2, the compounds marked with an asterisk (*), such as Quercetin, Kaempferol, and Coumarin, adhere to Lipinski's Rule of Five, as they exhibit one or no violations (≤ 1). These compounds are predicted to possess favorable physicochemical properties conducive to good absorption and permeability, making them promising candidates for oral drug delivery.

Table 1. Metabolic identification results of combined corn silk and jasmine flower extracts using UPLC-QToF-MS/MS

Peak	Retention Time (RT)	% Area	Measured ion Mass	Calculated ion Mass	Ion Formula $[M-H]^+$	Compound and Structure	Group
01	1.261	6.38	381.0793	381.0822	$[C17H17O10]^+$	9-Hydroxy-7-oxo-7H-furo[3,2-g]chromen-4-yl β-D-glucopyranoside	Coumarin
02	1.261		365.1067	365.1084	$[C14H21O11]^+$	2,3,4,5-Tetra-O-acetylhexonic acid	Asam karbosilat
03	1.562		229.1565	229.1552	$[C11H21N2O3]^+$	L-prolyl-L-leucine	protein
04	1.562		276.1460	276.1447	$[C12H22NO6]^+$	O-Glutarylcarnitine	acyl carnitines.
05	1.562		294.1565	294.1566	$[C13H20N5O3]^+$	2-(3,4-Dimethoxy-benzylamino)-1-(2-methyl-2H-tetrazol-5-yl)-ethanol	alkohol
06	2.181	0.10	289.0934	289.0923	$[C12H17O8]^+$	Glucosylisomaltol; 1-(3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}furan-2-yl)ethan-1-one	Glycoside/ Sugar group
07	2.575	0.80	328.1402	328.1396	$[C15H22NO7]^+$	N-(1-Deoxy-1-fructosyl)phenylalanine	Phenylalanine and derivatives
08	2.575		310.1296	1310.250	$[C10H20N3O8]^+$	citrulline malate	Malate acid
09	3.433	0.17	147.0456	147.0446	$[C9H7O2]^+$	Coumarin; 1-Benzopyran-2-one	coumarins and derivatives
10	3.671	1.08	367.1514	367.1545	$[C22H23O5]^+$	curcumin II; monodemethoxycurcumin	methoxyphenols
11	3.981		490.2286	490.2277	$C27H32N5O2S]^+$	2-[(3-sec-Butyl-4-oxo-3,4-dihydro-2-chinazolinyl)sulfanyl]-N-[3-(2-methyl-2-propanyl)-1-phenyl-1H-pyrazol-5-yl]acetamid	acetamida
12	4.445	4.35	757.2169	757.2191	$[C33H41O20]^+$	Quercetin 3-O-rhamnosyl-(1->2)-rhamnosyl-(1->6)-glucoside; Quercetin-3-neohesperidoside-7-rhamnoside	flavonoid-3-o-glycosides
13	4.445		611.1609	611.1612	$[C27H31O16]^+$	Rutin; Quercetin-3-O-rutinoside; 3-Rhamnoglucosylquercetin	flavonoid-3-o-glycosides
14	4.445		303.0510	303.0505	$[C15H11O7]^+$	Quercetin; 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chromen-4-one	flavonols
15	4.462		741.2224	741.2242	$[C33H41O19]^+$	Robinin; Kaempferol 3-O-beta-robinoside 7-O-alpha-L-rhamnopyranoside	flavonoid-7-o-glycosides
16	4.462		595.1664	595.1663	$[C27H31O15]^+$	Kaempferol 3-neohesperidoside; 5,7-Dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl 2-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranoside	flavonoid-3-o-glycosides

17	4.462		287.0564	287.0565	$[C_{15}H_{11}O_6]^+$	Kaempferol; 3 4′ 5 7-tetrahydroxyflavone	Flavonols
18	4.973	1.67	411.2012	411.2019	$[C_{21}H_{31}O_8]^+$	Pteroside A; 2-[(2*S*)-2-(Hydroxymethyl)-2,4,6-trimethyl-3-oxo-2,3-dihydro-1H-inden-5-yl]ethyl-β-D-glucopyranosid	glycoside
19	4.973		565.1545	565.1557	$[C_{26}H_{29}O_{14}]^+$	Apiin; Apigenin-7-apioglucoside	flavone apigenin / Flavonolid
20	5.655	1.62	593.1877	593.1870	$[C_{28}H_{33}O_{14}]^+$	Margaritene; 2″-O-α-rhamnosyl-4′-O-methylvitexin	flavonoid 8-c-glycosides
21	6.358	14.56	617.2585	617.2598	$[C_{32}H_{41}O_{12}]^+$	javanicin D; 1S,2R,3S,3aR,5S,6aR,7aR,10S,11aS,11bS,11cR)-2,10-Diacetoxy-3-hydroxy-5-methoxy-3,11a,11c-trimethyl-11-oxohexadecahydrodibenzo[de,g]chromen-1-yl 1,3-benzodioxole-5-carboxylate	benzodioxol-5-carboxylat
22	6.638	3.55	591.1687	591.1714	$[C_{28}H_{31}O_{14}]^+$	3'-O-Methylmaysin	flavonoid c-glycosides
23	6.638		445.1152	445.1135	$[C_{22}H_{21}O_{10}]^+$	Rothindin; Pseudobaptigenin 7-O-glucoside	isoflavonoid o-glycosides
24	6.638		609.1793	609.1819	$[C_{28}H_{33}O_{15}]^+$	Diosmin; Diosmetin 7-b-Rutinoside	flavonoid-7-o-glycosides
25	7.341	1.30	823.3152	823.3155	$C_{26}H_{55}N_4O_{25}]^+$	(3β,15β,16α,17β)-21-Oxo-16-vinyl-19,20-didehydro-18-oxayohimban-17-yl β-D-glucopyranosyl-(1->6)-β-D-glucopyranosyl-(1->2)-β-D-mannopyranoside	glycoside
26	8.116	0.25	601.2657	601.2649	$[C_{32}H_{41}O_{11}]^+$	Swietemahonin B; (1R,2R,4S,5R,9R,10R,13R,14S,15S,17R)-15-[(1R)-1-Acetoxy-2-methoxy-2-oxoethyl]-9-(3-furyl)-10,14,16,16-tetramethyl-7,18-dioxo-3,8-dioxapentacyclo[12.3.1.0~2,4~.0~4,13~.0~5,10~]octadec-17-yl propionate	Limonoids
27	8.614	0.61	443.0972	443.0978	$[C_{22}H_{19}O_{10}]^+$	(−)-Epicatechin-3-O-gallate; 2*R*,3*R*)-3′,4′,5,7-Tetrahydroxyflavan-3-yl 3,4,5-trihydroxybenzoate	catechin gallates (flavonoid)
28	9.057	0.41	557.1656	557.1661	$[C_{28}H_{29}O_{12}]^+$	5-Hydroxy-2-(4-methoxy-2-oxo-2H-pyran-6-yl)-3-methylphenyl 2-O-[(2E)-3-(4-hydroxyphenyl)-2-propenoyl]-β-D-glucopyranoside	Glycoside (sugar group)
29	9.338	0.07	310.2382	310.2382	$[C_{18}H_{32}NO_3]^+$	3-Oxo-dodecan-(2-amino-cyclohexanone)	Lipid
30	9.823	0.12	327.0871	327.0869	$[C_{18}H_{15}O_6]^+$	Dihydrosterigmatocystin; 1,2-Dihydro-6-methoxy-7-hydroxyfuroxanthone	xanthone
31	9.915	0.12	403.1393	403.1393	$[C_{21}H_{23}O_8]^+$	Nobiletin; 5,6,7,8,3',4'-Hexamethoxyflavone	8-o-methylated flavonoids

32	10.175	0.45	343.2967	2343.961	$[C19H39N2O3]^+$	cocamidopropyl betaine; Lauramidopropyl betaine	Lipid
33	10.175		240.2343	240.2327	$[C15H30NO]^+$	N-Dodecyl-2-propenamide	Lipid
34	10.547	0.05	373.1289	373.1287	$[C20H21O7]^+$	Tangeritin; 4′,5,6,7,8-Pentamethoxyflavone	8-o-methylated flavonoids
35	10.949	0.10	214.2545	214.2535	$[C14H32N]^+$	Dimethyl Lauramine	Lipid
36	11.673	0.73	518.3245	518.3230	$[C28H44N3O6]^+$	N-[(trans-4-{[(N-{[(2-Methyl-2-propanyl)oxy]carbonyl}-L-leucyl)amino]methyl}cyclohexyl)carbonyl]-L-phenylalanin	Asam amino2 (protein)
37	11.911	4.38	518.3237	518.3230	$[C28H44N3O6]^+$	N-[(trans-4-{[(N-{[(2-Methyl-2-propanyl)oxy]carbonyl}-L-leucyl)amino]methyl}cyclohexyl)carbonyl]-L-phenylalanin	Asam amino2 (protein)
38	12.418	2.72	520.3395	520.3387	$[C28H46N3O6]^+$	Boc-3-(Z-amino)-L-alanine (dicyclohexylammonium) salt	Salt amino acid
39	12.685	11.81	520.3389	520.3387	$[C28H46N3O6]^+$	Boc-3-(Z-amino)-L-alanine (dicyclohexylammonium) salt	Salt amino acid
40	13.276	3.19	496.3409	496.3387	$[C26H46N3O6]^+$	(2R,4S,5S,7S)-5-Amino-N-(3-amino-3-oxopropyl)-4-hydroxy-7-[4-methoxy-3-(3-methoxypropoxy)benzyl]-2,8-dimethylnonanamide	Lipid
41	13.606	1.87	522.3547	522.3543	$[C28H48N3O6]^+$	N-{[(2-Methyl-2-propanyl)oxy]carbonyl}-L-phenylalanyl-N-[(2S,3R)-2-hydroxy-1-isobutoxy-5-methyl-3-hexanyl]-L-alaninamide	Lipid
42	14.941	17.28	610.5419	610.5410	$[C37H72NO5]^+$	N-(1,1-Dihydroxy-3-methyl-1-buten-2-yl)-2-{[(1E)-1-hydroxy-1-hexadecen-1-yl]oxy}hexadecanamide	Lipid
43	16.326	0.15	780.5514	780.5512	C40H83N3O5S2P	No Information	No Information
44	17.121	20.20	575.5051	575.5039	$[C37H67O4]^+$	Montecristin ; 3-[(11S,12S,15Z,19Z)-11,12-Dihydroxy-15,19-dotriacontadien-1-yl]-5-methyl-2(5H)-furanone	(waxy derivatives of fatty acid)/ Lipid

Table 2. Lipinski's Rule of Five parameters for bioactive compounds

Bioactive Compounds	Lipinski's Rule of Five Parameters					Violation of Lipinski's Rule ≤ 1
	Molecular Weight (<500 Da)	mlog P (<5)	H-Bond Donors (<5)	H-Bond Acceptors (<10)	Rotatable Bonds (40-130)	
Quercetin*	371.52	6	0	2	119.72	1
Robinin	740.66	-2.89	11	18	170.32	4
Kaempferol*	286.24	-0.03	4	6	76.01	0
Rutin	610.52	-1.69	10	15	141.38	4
Coumarin (1-Benzopyran-2-one)*	259.3	2.84	0	3	76.5	0
Nobiletin*	402.4	3.51	0	7	106.87	0
Tangeritin	372.4	3.5	0	6	100.38	0

(pentametoksiflavon)*						
Monodemethoxycurcumin (curcumin II)*	338.4	3.36	2	5	96.31	0
Epicatechin-3-O-gallate	442.4	2.53	7	10	110.04	2
Chlorogenic acid*	354.31	-0.65	6	9	83.5	0
Apiin	564.5	-1.49	8	13	132.56	4
Margaritene	592.5	-0.75	8	13	142.3	4
Javanicin D	616.7	2.96	1	12	151.51	3
Rothindin*	444.4	0.37	4	9	108.3	0
Glibenclamide*	494	5.9	3	8	126.25	0

** Fulfilling Lipinski's Rule*

Table 3. The Root Mean Square Deviation (RMSD) of ligands with targets GLP-1, IGF, GLUT4, α-glucosidase, SOD

Ligands	GLP-1	IGF	GLUT4	α-glucosidase	SOD
Quercetin	22.34	1.43	2.69	1.54	1.36
Chlorogenic acid	3.62	1.72	2.61	2.47	2.52
Coumarin (1-Benzopyran-2-one)	1.53	2.70	1.67	1.70	2.12
Kaempferol	2.87	1.67	3.55	1.87	1.29
Monodemethoxycurcumin (curcumin II)	2.58	2.55	23.44	2.2	1.50
Nobiletin	1.49	1.83	1.99	3.35	0.79
Rothindin	2.27	1.20	2.68	1.67	2.16
Tangeritin (pentametoksiflavon)	1.87	1.16	2.76	1.33	2.20
Glibenclamide*	3.18	1.87	4.11	3.10	1.65

** Types of drugs used for diabetes mellitus.*

Table 4. Ligands and number of hydrogen bond residues for targets GLP-1, IGF, GLUT4, α-glucosidase, SOD

Ligands	Number of hydrogen bond residues				
	GLP-1	IGF	GLUT4	α-glucosidase	SOD
Quercetin	4	4	2	4	2
Chlorogenic acid	4	3	5	5	2
Coumarin (1-Benzopyran-2-one)	0	1	1	1	2
Kaempferol	4	2	2	3	3
Monodemethoxycurcumin (curcumin II)	3	-	2	1	3
Nobiletin	4	3	4	4	4
Rothindin	5	2	5	3	4
Tangeritin (pentametoksiflavon)	3	3	4	2	4
Glibenclamide*	4	2	3	0	2

** Types of drugs used for diabetes mellitus.*

Molecular docking analysis based on the Root Mean Square Deviation (RMSD) of the ligand-protein complex was performed to assess binding stability, with values below 2.0 Å considered to indicate a stable interaction (Table 3). Nobiletin exhibited the broadest stability profile, forming stable complexes with GLP-1 (1.496 Å), IGF (1.835 Å), GLUT4 (1.991 Å), and SOD (0.797 Å). The reference compound, glibenclamide, met the stability criteria only for IGF (1.872 Å) and SOD (1.656 Å).

Based on the results of the molecular docking simulation presented in Figure 2, the ligand rohitin (7) demonstrated the highest and most stable binding affinity specifically toward the target protein GLUT4 (▲), with a value of -9.9 kcal/mol. In addition, several other ligands, such as quercetin (1) and tangeretin (8), showed strong potential interactions with other target proteins, particularly IGF and GLP-1, although not as strong as the interaction between othindin and GLUT4.

The molecular interactions between the nine ligands and five protein targets (GLP-1, IGF, GLUT4, α-glucosidase, and SOD) were measured (Tables 4 and 5). Many ligands have strong

interaction potentials; for example, Rothindin and Chlorogenic Acid have a large number of hydrogen bonds, five for both GLP-1/GLUT4 and GLUT4/α-glucosidase. In contrast, only a small number of hydrogen bonds were observed in most coumarin targets, indicating a lower binding energy. The standard drug, glibenclamide, showed moderate interactions with GLP-1, IGF, and GLUT4; however, no hydrogen bond formation was observed with α-glucosidase. Overall, these results suggest that ligands such as rotopin, chlorogenic acid, and quercetin are promising candidates for modulating these biological targets, as the number of hydrogen bonds is a key indicator of stable ligand-protein binding. Table 5 shows that rothindin and GLUT 4 protein form conventional hydrogen bonds with the amino acids GLN A:188, ASN A:57, and THR A:322. This explains the superior binding affinity of rohtindin compared to that of the other compounds for GLUT 4. This comparative study highlights the distinct potential of each phytochemical to target specific proteins in cancer cells. While rothin excels in its interactions with GLUT 4, GLP-1, and SOD, Quercetin demonstrates a strong binding affinity for IGF protein, with a ΔG value of -8.7 kcal/mol.

Rothindin with GLUT4 and GLP-1

Rothindin is an organic compound belonging to the class of isoflavonoid O-glycosides, which are O-glycosylated derivatives of natural isoflavonoids derived from the 3-phenylchromen-4-one structure (FooDB, 2019). Rothindin has been tentatively identified as a flavonoid in oolong tea extracts (Fraser et al., 2014). This identification was based on an accurate mass match with the molecular formula of $C_{22}H_{20}O_{10}$ found in the metabolite database (Fraser et al., 2014). Other studies have shown that rothindin is one of the seven main isoflavonoid compounds successfully identified and isolated from the extracts of *Trifolium pratense L.* (red clover). The rothindin found in this study acts as a potent inhibitor of the cyclooxygenase-2 (COX-2) enzyme. Inhibition of COX-2 activity can reduce the production of prostaglandins, which triggers inflammation and cancer cell growth (Hou et al., 2019).

Although specific studies on the interactions of rohtindin with diabetes-related targets are limited, they are known to form hydrogen bonds with proteins such as GLUT4 and GLP-1. GLUT4 is a glucose transporter involved in the regulation of glucose uptake in response to insulin, making it a potential target for diabetes treatment (T. Wang et al., 2020). GLP-1 (glucagon-like peptide-1) is an incretin hormone that enhances insulin secretion (Zheng et al., 2024). Rothindin is a compound found in M. caesia fruit extract, which exhibits the strongest free radical scavenging antioxidant activity compared to the seven other fruit extracts tested, but it has weak α-glucosidase inhibitory activity (Mohamed et al., 2021).

Although specific studies on the direct antidiabetic effects of rothindin are limited, its mechanisms of action involve interactions with key glucose-regulatory proteins. Rothindin forms hydrogen bonds with GLUT4, an insulin-responsive glucose transporter, and GLP-1, an incretin hormone that promotes insulin secretion. Although exhibiting only weak α-glucosidase inhibitory activity, rothindin also acts as a potent COX-2 inhibitor, suggesting a potential anti-inflammatory pathway associated with insulin resistance.

Chlorogenic Acid with GLUT4 and α glucosidase

Chlorogenic Acid has shown the capability forms hydrogen bonds with GLUT4 and α-glucosidase. Interaction with GLUT4 suggests its role in improving glucose uptake, whereas α-glucosidase, an enzyme involved in carbohydrate digestion, has the potential to reduce postprandial blood glucose levels. Chlorogenic acid has been studied for its antidiabetic potential, although much of its insecticidal activity against Spodoptera frugiperda has been reported (Herrera-Mayorga et al., 2022; Nabil-Adam et al., 2023). Chlorogenic acid (CGA) is a bioactive compound that forms noncovalent interactions with target proteins, including hydrogen bonding, and plays a significant role in its inhibitory effects on enzymes, such as α-glucosidase. The mechanism by which CGA interacts with α-glucosidase primarily involves the spontaneous formation of hydrogen bond complexes. This interaction leads to changes in the secondary structure of the enzyme, thereby affecting its activity (Xing et al., 2021). Chlorogenic acid is a polyphenol compound widely found in plants, such as green coffee beans, with the molecular formula $C_{16}H_{18}O_9$. It has various therapeutic functions, including anti-inflammatory and antioxidant effects, and is associated with the management

of diabetes mellitus via its role in maintaining glucose homeostasis, reducing glucose absorption and release, and enhancing insulin secretion (Nguyen et al., 2024).

Liquid Chromatography-Mass Spectrometry (LC-MS) analysis has shown that corn silk samples contain five types of chlorogenic acids (CGA) (Patel et al., 2023). Chlorogenic acids are esters of hydroxycinnamic acids, such as caffeic, p-coumaric, and quinic acids (Rahman & Wan Rosli, 2014; Ren et al., 2009). Other studies have shown that chlorogenic acid improves diabetic conditions in mice by activating AMPK, which significantly increases the expression of GLUT-4 in skeletal muscles, thereby facilitating GLUT-4 translocation to enhance glucose uptake(Jin et al., 2015). Regarding the GLUT4 protein, the docking simulations and in vitro studies have suggested that certain natural compounds, including those similar to chlorogenic acid, may interact with the GLUT4 transporter via hydrogen bonds, which enhances the stability of the formed complexes and influences glucose uptake (Sonia et al., 2025).

For α-glucosidase, molecular docking studies have simulated the binding of chlorogenic acid to specific amino acid residues in the enzyme's active site, suggesting that the binding is facilitated through hydrogen bonds with residues such as Lys-156, Ser-157, Gly-160, and others, leading to the stabilization of the enzyme-inhibitor complex (Dong et al., 2021). Other studies have shown that chlorogenic acid can inhibit the activity of α-glucosidase through a complex mechanism, including mixed inhibition (competitive and non-competitive), competitive inhibition, and denaturing effects that can damage the structure of the enzyme (Abioye et al., 2023). Although its activity is relatively weak, chlorogenic acid exhibits a strong synergistic effect when combined with the antidiabetic drug acarbose, resulting in greater inhibitory power (Abioye et al., 2023). In addition, chlorogenic acid reversibly inhibits α-glucosidase activity through a mixed-type mechanism by binding to residues within the enzyme's active pocket via hydrogen bonding and hydrophobic interactions, resulting in conformational changes in the enzyme (Jiang et al., 2025).

Chlorogenic acid (CGA) exerts mechanisms relevant to glucose control by targeting glucose absorption and peripheral uptake. It inhibits α-glucosidase through a mixed-type inhibition mechanism by binding to the active site of the enzyme via hydrogen bonds, thereby delaying carbohydrate digestion. CGA promotes glucose disposal by activating the AMPK pathway, which subsequently enhances the expression and translocation of the GLUT4 transporter in skeletal muscles.

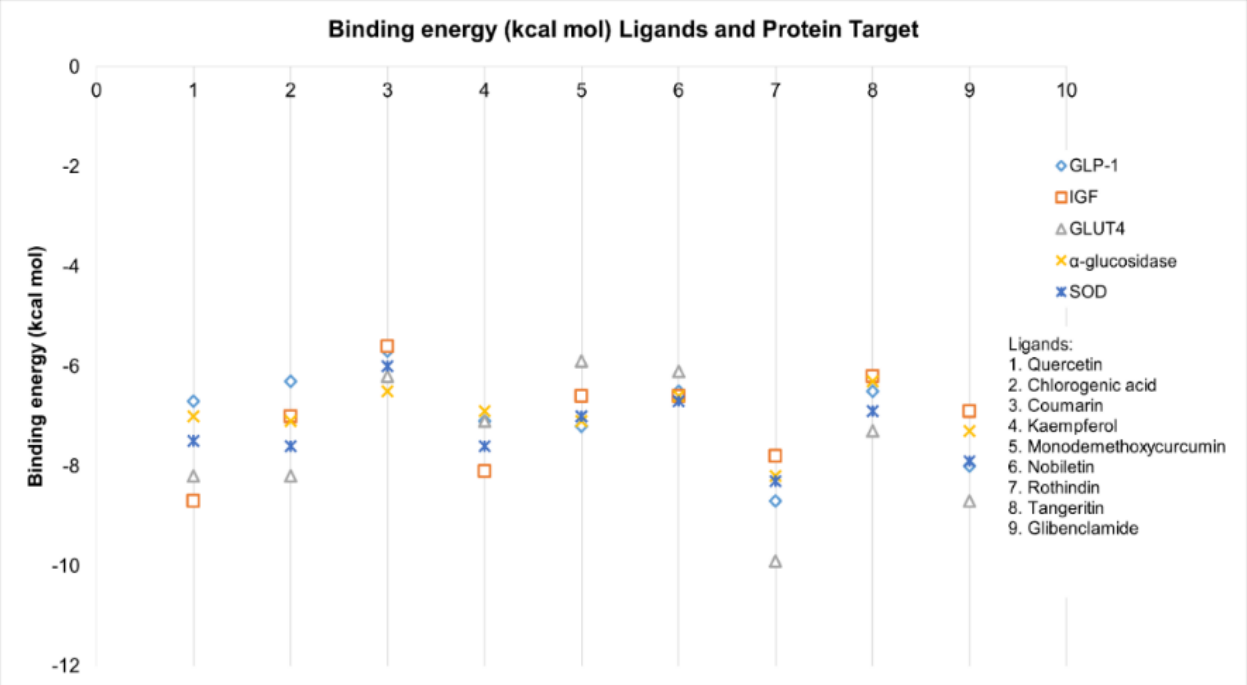
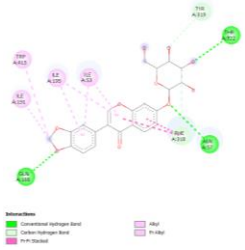
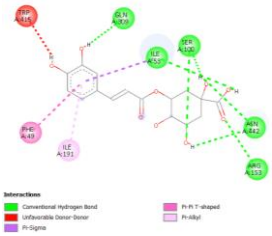
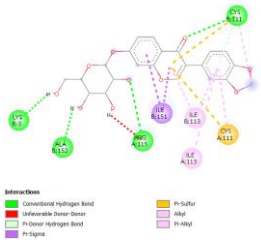
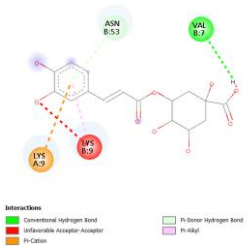
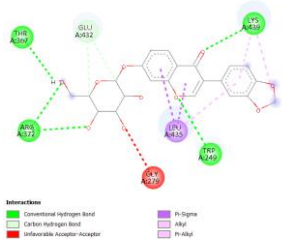
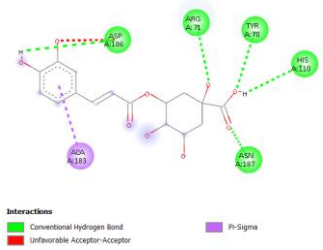


Figure 2. Binding energy (kcal mol) Ligands and protein targets.

Table 5. Molecular docking results and visualizations of corn silk and jasmine flower phytochemicals with the proteins based on binding affinity and hydrogen bond

Ligan — Protein (ΔG), 2D Visualization	
Rothindin — GLUT4 (ΔG: −9.9)	Chlorogenic acid — GLUT4 (ΔG: −8.2)
	
Glutamina (Gln, Q), Fenilalanina (Phe, F), Asparagina (Asn, N), Tirosina (Tyr, Y), Treonina (Thr, T)	Glutamina (Gln, Q), Isoleusina (Ile, I), Serina (Ser, S), Arginina (Arg, R)
Rothindin — SOD (ΔG: −8.3)	Chlorogenic acid — SOD (ΔG: −7.6)
	
Lisina (Lys, K), Alanina (Ala, A), Arginina (Arg, R), Sisteina (Cys, C)	Valina (Val, V), Asparagina (Asn, N)
Rothindin — GLP-1 (ΔG: −8.7)	Chlorogenic acid — α-Glucosidase (ΔG: −7.1)
	
Arginina (Arg, R), Treonina (Thr, T), Asam glutamat (Glu, E), Lisina (Lys, K), Triptofan (Trp, W)	Asam aspartat (Asp, D), Arginina (Arg, R), Tirosina (Tyr, Y), Histidina (His, H), Asparagina (Asn, N)

Quercetin with IGF-1 (Insulin-like Growth Factor 1)

Quercetin exhibits a strong binding affinity for IGF-1 (Insulin-like Growth Factor 1), which is relevant for diabetes management. Studies in rats have shown that diabetes causes a significant decrease in the expression of insulin-like growth factor-1 (IGF-1) in the hippocampus, which is associated with insulin deficiency (Ola et al. 2014). Administration of quercetin (QC), either in its pure form or conjugated with superparamagnetic iron oxide nanoparticles (QCSPIONs), significantly restored IGF-1 mRNA expression in diabetic rats (Dini et al., 2021). Quercetin, through its antioxidant and anti-inflammatory properties, supports insulin signaling pathways, which may indirectly influence IGF-1 activity in the liver. Quercetin has been shown to ameliorates insulin resistance and improves glucose homeostasis by modulating various metabolic and inflammatory pathways (Ansari et al., 2022). This comprehensive effect on glucose metabolism suggests that quercetin is beneficial for managing diabetes and potentially enhances IGF-1-mediated pathways.

The combined extract of corn silk and jasmine flowers contains a diverse array of bioactive compounds, including flavonoids, lipids, amino acids, glycosides, coumarins, and organic acids. These compounds interact with multiple diabetes-related targets, including GLUT4, GLP-1, IGF-1, α-glucosidase, and SOD. Key components, such as othindin, chlorogenic

acid, and quercetin, demonstrate potential antidiabetic effects through various mechanisms. Rothindin forms hydrogen bonds with GLUT4 and GLP-1, potentially influencing glucose uptake and insulin secretion. Chlorogenic Acid interacts with GLUT4 and α-glucosidase, suggesting its role in improving glucose uptake and reducing postprandial blood glucose levels. Quercetin has a strong binding affinity for IGF-1 and supports insulin signaling pathways. This synergistic combination of bioactive compounds offers promising therapeutic potential for the management of diabetes through multiple molecular targets.

The ability of the extract to simultaneously modulate multiple key diabetes-related pathways indicates its potential as a source for developing integrated nutraceuticals or functional foods designed to support glycemic management. The limitation of this study lies in its nature as an in silico study; therefore, the results of the interactions between bioactive compounds and diabetes target proteins were based solely on computational predictions. Further experimental validation is necessary to confirm these findings, including in vitro and in vivo testing, to evaluate the antidiabetic effects of the combination of corn silk and jasmine flower extracts.

Conclusion

The combined extract of corn silk (*Zea mays L.*) and jasmine flowers (*Jasminum sambac*) has shown promising antidiabetic potential in previous studies. LC-MS/MS analysis successfully identified 44 bioactive compounds, with several major compounds, such as othindin, chlorogenic acid, and quercetin, demonstrating strong binding affinities to diabetes-related target proteins, such as GLUT4, GLP-1, IGF-1, and α-glucosidase. Rothindin showed the highest affinity for GLUT4, with a binding energy of -9.9 kcal/mol. These molecular interactions suggest the potential of the combined extract to modulate various glucose metabolic pathways relevant to diabetes. Although these findings provide a strong foundation for the development of food-based antidiabetic therapies, further experimental validation through in vitro and in vivo studies is required to confirm their effectiveness and safety of these compounds.

Acknowledgments

The authors gratefully acknowledge the financial support provided by the Indonesian Education Scholarship from the Center for Higher Education Funding and Assessment, Ministry of Higher Education, Science, and Technology of the Republic of Indonesia, and the Endowment Fund for the Education Agency, Ministry of Finance of the Republic of Indonesia

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