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Unraveling the antidiabetic and antidepressant effects of crude methanolic extracts of *Clitoria ternetea* flower in diabetic mice

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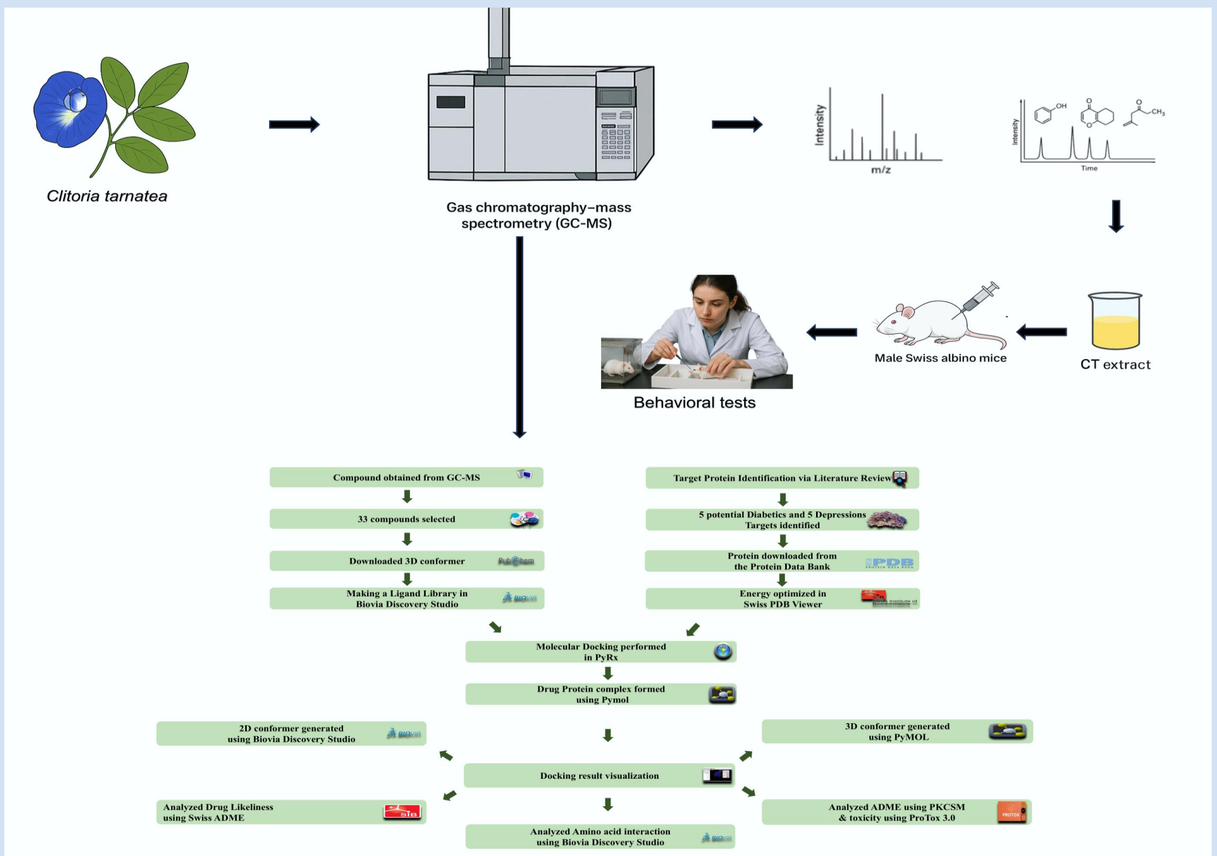
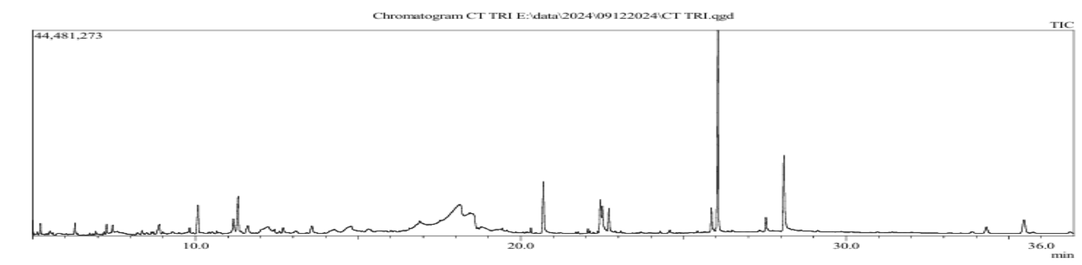
INTRODUCTION & AIM

Clitoria ternatea L. (CT), commonly known as the butterfly pea or Asian pigeonwings, is a perennial herbaceous plant belonging to the family Fabaceae. It is widely distributed in tropical and subtropical regions of Asia and is easily recognized by its striking deep-blue flowers. Traditionally, *C. ternatea* has been used in Ayurvedic and folk medicine for its diverse therapeutic properties, including memory enhancement, anti-inflammatory, antioxidant, anxiolytic, and neuroprotective effects [1]. Its roots, leaves, and flowers are known to contain a rich profile of bioactive phytochemicals such as flavonoids, alkaloids, steroids, tannins, and glycosides, which contribute to its broad pharmacological potential. Despite extensive traditional use, scientific exploration of its efficacy in complex metabolic and neurological disorders, particularly diabetes and depression. Both conditions are often interlinked through oxidative stress and neuroendocrine dysregulation, highlighting the need for multifunctional plant-based therapeutic agents. The present study was therefore designed to isolate and characterize bioactive compounds from C. ternatea using gas chromatography–mass spectrometry (GC-MS) and to evaluate their antidiabetic and antidepressant potential through a combination of in silico, in vitro, and in vivo approaches. Molecular docking was performed to predict the interaction of isolated compounds with key antidiabetic and antidepressant protein targets, while in vivo studies on Swiss albino mice assessed pharmacological effects via blood glucose analysis and behavioral tests. Additionally, physicochemical profiling, drug-likeness, and ADMET analyses were conducted to predict pharmacokinetic suitability [2]. The aim of this study is to explore the phytochemical constituents of *Clitoria ternatea* and investigate their potential antidiabetic and antidepressant activities through a multifaceted approach integrating computational, biochemical, and behavioral analyses.

METHOD



RESULTS & DISCUSSION



Quantitative Result Table

ID#	Name	R.Time	m/z	Area	Height	Conc.	Similarity
1	2-Propanol, 1,1'-oxybis-	5.147	89.00	522356	231416	0.633	88
2	2-Furanmethanol	5.231	98.00	1097724	523042	1.330	96
3	Cyclohexanone	5.424	55.00	435530	157810	0.528	87
4	Ethanamine, 2-methoxy-N-(2-methoxyethyl)-N	5.524	102.00	1570506	316162	1.902	88
5	2(1H)-Pyrazinone	5.611	96.00	283603	153492	0.344	71
6	6-Oxa-bicyclo[3.1.0]hexan-3-one	6.295	98.00	2360920	1020425	2.860	96
7	Ethanone, 1-(6-methyl-7-oxabicyclo[4.1.0]hep	6.757	95.00	132638	73010	0.161	90
8	Imidazole, 1,4,5-trimethyl-	6.937	110.00	639050	259456	0.774	93
9	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-on	7.184	101.00	337538	174759	0.409	88
10	2-Oxopentanedioic acid	7.266	101.00	1300639	637658	1.576	94
11	1,2-Cyclooctanedione	7.452	55.00	805087	382708	0.975	87
12	Heptanoic acid, 6-hydroxy-, ethyl ester	8.350	102.00	435767	202953	0.528	88
13	Thymine	8.899	126.00	5031315	952335	6.095	96
14	N-Nitroso-2-methylthiazolidine	9.816	102.00	696141	242400	0.843	87
15	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-on	10.076	144.00	3719832	1250828	4.506	98
16	Benzofuran, 2,3-dihydro-	11.165	120.00	1230564	615191	1.491	89
17	5-Hydroxymethylfurfural	11.313	97.00	9824526	2736563	11.901	98
18	Dimethyl dl-malate	11.609	103.00	4699373	830828	5.693	93
19	Heptyl caprylate	12.702	115.00	701188	186372	0.849	87
20	3-Cyclopentylpropionic acid, 1-(cyclopentyl)et	13.592	84.00	1074022	236058	1.301	87
21	l-(+)-Ascorbic acid 2,6-dihexadecanoate	20.698	73.00	3588000	1063472	4.346	100
22	18-Methyl-nonadecane-1,2-dio, trimethylsilyl	21.759	73.00	167783	92584	0.203	71
23	Ethanol, 2-(9,12-octadecadienyloxy)-, (Z,Z)-	22.065	67.00	191192	96872	0.232	90
24	3-Tetradecanynoic acid	22.126	79.00	105218	52108	0.127	83
25	Linoelaidic acid	22.448	67.00	2239229	758040	2.712	95
26	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	22.507	79.00	1674179	534710	2.028	81
27	i-Propyl 16-methyl-heptadecanoate	22.709	73.00	1091517	389013	1.322	96
28	Glycerol 1-palmitate	25.859	98.00	979801	429139	1.187	97
29	Di-n-octyl phthalate	26.062	149.00	25408454	8213101	30.778	99
30	2- Bromopropionic acid, tridecyl ester	27.536	57.00	506745	199587	0.614	92
31	13-Docosenamide, (Z)-	28.090	59.00	8917216	2570998	10.802	98
32	Stigmasterol	34.316	55.00	372560	71181	0.451	88
33	.gamma.-Sitosterol	35.472	57.00	413287	72354	0.501	94

Fig: Isolated compounds from *Clitoria tarnatea* by GC-MS.

Behavioral Tests on Diabetic induced Mice:

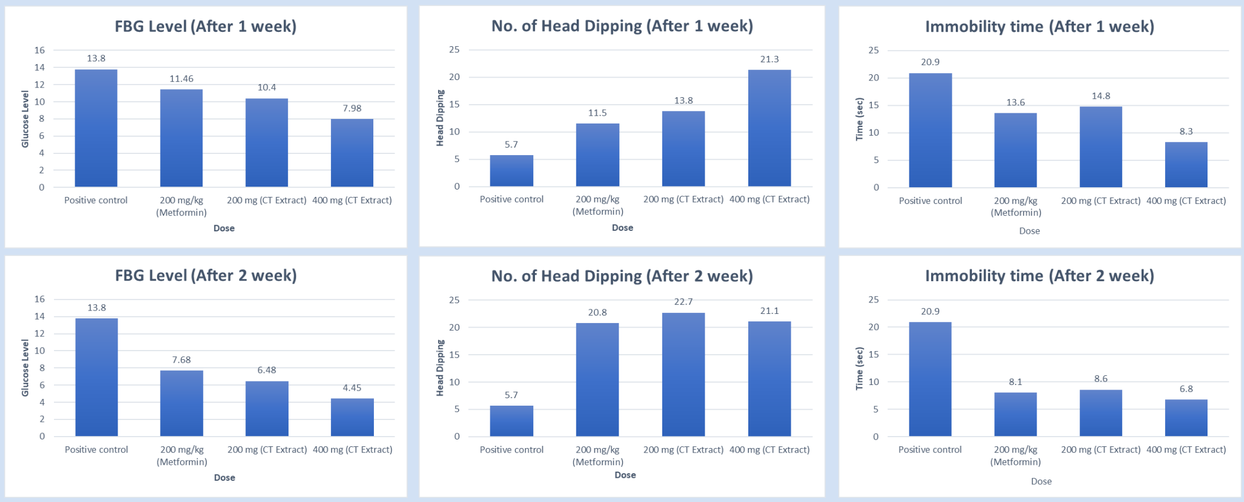


Table 1. Docking score (kcal/mol) of the top 2 compounds against 5 Diabetic targets.

Ligand	Binding affinity				
	Targets				
	PPAR GAMMA	DPP4	SGLT2	AMPK	GLP-1 receptor
	2PRG	6BE1	7VSI	4QFG	5VEW
Stigmasterol	-7	-8.4	-8.9	-8.3	-9.1
Gamma-Sitosterol	-7.2	-8	-9	-7.8	-8.9
Metformin(Standard)	-4.9	-4.7	-4.6	-4.8	-4.6

Table 2. Docking score (kcal/mol) of the top 2 compounds against 5 Depression targets.

Ligand	Binding affinity				
	Targets				
	MAO B	DOPAMIN D2	DOPAMIN D3	GABA	5-HT
	2V5Z	6LUQ	3PBL	4COF	7VOD
Stigmasterol	-9.8	-7.9	-8.3	-7.7	-10.5
Gamma-Sitosterol	-9.7	-7.8	-7.8	-7.5	-10.3
Clonazepam(Standard)	-7.4	-7.4	-7.9	-7.7	-9
Citalopram(Standard)	-8	-6.7	-6.7	-6.7	-9

Table 3. ADME analysis of the compounds with promising binding affinity.

Properties	Model name (Unit)	Compound	
		Stigmasterol	gamma-Sitosterol
Absorption	Water solubility (log mol/L)	-6.682	-6.773
	Caco2 permeability (log Papp in 10-6 cm/s)	1.213	1.201
	Intestinal absorption (human) (% Absorbed)	94.97	94.464
	Skin Permeability (log Kp)	-2.783	-2.783
	P-glycoprotein substrate	No	No
	P-glycoprotein I inhibitor	Yes	Yes
	P-glycoprotein II inhibitor	Yes	Yes
Distribution	VDss (human) (log L/kg)	0.178	0.193
	Fraction unbound (human) (Fu)	0	0
	BBB permeability	0.771	0.781
	CNS permeability	-1.652	-1.705
Metabolism	CYP2D6 substrate	No	No
	CYP3A4 substrate	Yes	Yes
	CYP1A2 inhibitior	No	No
	CYP2C19 inhibitior	No	No
	CYP2C9 inhibitior	No	No
	CYP2D6 inhibitior	No	No
	CYP3A4 inhibitior	No	No
Excretion	Total Clearance (log ml/min/kg)	0.618	0.628
	Renal OCT2 substrate	No	No

Table 5. Amino acid interaction analysis of the top 2 hits.

Sl No	Ligand	Target	Binding Affinity (kcal/mol)	H-bond(Å)	Hydrophobic Interactions and Other Interactions
1	Stigmasterol	2PRG	-7		ILE328A(4.81), PRO358A(5.06), LEU279B(4.83,3.91), LEU354A(4.22), VAL331A(4.85), VAL332A(5.47), ILE286B(4.72), LEU354A(5.00), PHE324A(5.12, 5.42), PHE347A(4.72)
		6BE1	-8.4	VAL207A(2.68)	PHE357A(3.47), TYR547A(3.75, 3.72), LYS554A(5.04,4.89), PHE357A(5.08), PHE357A(4.04, 4.74)
		7VSI	-8.9		ALA90A(5.26, 4.01, 3.77), VAL95A(4.14), LEU274A(4.04), LEU84A(4.92), VAL95A(5.03), PHE98A(4.69), PHE453A(5.27)
		4QFG	-8.3		ALA434A(4.17), LEU146A(4.99), VAL30A(3.57), LEU22A(4.40), LEU146A(4.47, 4.88), VAL96A(4.67), TYR95A(4.80)
		5VEW	-9.1		ILE328A(5.42, 4.32), PRO358A(4.77), LEU278B(5.06), LEU279B(5.35, 5.27, 3.58), LEU354A(4.35, 4.97), VAL331A(4.59), PHE324A(5.13, 4.85), PHE347A(4.31)
		2V5Z	-9.8		VAL106B(4.35), PRO105B(4.96), PHE103B(4.68, 4.17, 4.66), TYR112B(4.99), HIS115B(5.15), TRP119B(5.07)
		6LUQ	-7.9		VAL315A(5.43, 4.06, 5.13), LYS390A(4.57), LYS391A(4.96, 4.12, 4.78), ARG219A(4.82), ARG220A(4.41, 3.70), TRP379A(5.35, 5.23)
		3PBL	-8.3		MET134A(4.44, 5.22), PRO135A(5.40), VAL136A(4.74), ILE1009A(4.88, 5.14, 4.56, 4.87), ARG219A(4.37, 4.97), LYS221A(4.55)
		4COF	-7.7		LYS103E(4.97, 4.71), LYS102E(4.01)
		7VOD	-10.5		VAL156A(5.05, 4.77, 4.10), LEU229A(4.93, 4.87), VAL366A(5.49, 5.06), VAL235A(3.82), ILE152A(4.42), TYR139A(5.06, 5.14), TRP151A(4.04, 5.15), PHE339A(5.42)
2	gamma-Sitosterol	2PRG	-7.2		PRO366A(5.12), PRO398B(4.48, 4.15), ILE445A(5.40), TYR477B(5.41)
		6BE1	-8	VAL207A(2.58)	PHE357A(3.47, 5.05, 4.08, 4.78), LYS554A(4.69), TYR547A(4.29, 3.79)
		7VSI	-9		PHE98A(3.79, 5.12, 3.94), ALA90A(4.86, 3.66, 3.84), VAL95A(4.40, 5.13), LEU274A(4.37), PHE453A(4.97)
		4QFG	-7.8		LEU146A(5.19, 4.68, 5.11), ALA156A(4.31, 3.76), LEU22A(4.23), VAL30A(4.58), MET93A(5.31), ILE77A(4.34)
		5VEW	-8.9		ILE328A(4.81), PRO358A(5.06), LEU279B(4.83, 3.91), LEU354A(4.22, 5.00), VAL331A(4.85, 4.10), VAL332A(5.47), ILE286B(4.72), PHE324A(5.12, 5.42), PHE347A(4.72)
		2V5Z	-9.7		PHE103B(3.82, 3.83, 5.11, 4.37, 4.03), ARG120B(4.03), ILE477B(5.49, 5.29), TYR112B(4.88), TRP119B(5.15, 4.70, 3.82)
		6LUQ	-7.8		ALA314A(3.50), VAL315A(5.15, 4.76, 4.65), LYS390A(4.66, 4.36, 4.32), LYS391A(4.80, 4.13), ARG220A(4.75, 3.75), TRP379A(4.59, 5.39)
		3PBL	-7.8		MET134A(4.65, 5.00, 5.18), VAL136A(4.62), ILE1009A(5.35, 5.15, 4.28, 4.72, 4.36), ARG1008A(4.70), VAL214A(5.26, 4.31), VAL133A(4.54)
		4COF	-7.5		LYS103A(4.99), LYS103B(5.42), LYS102B(4.02, 4.32), PHE105A(4.69)
		7VOD	-10.3		THR134A(2.10), ILE152A(5.17), VAL156A(5.50, 3.73), LEU229A(5.40), VAL366A(4.83, 4.60, 4.15), TRP151A(4.63, 5.33), PHE243A(4.43, 4.76), PHE339A(5.47), PHE340A(5.11)

Table 4. Toxicity analysis of top compounds

Compounds	LD50 (mg/Kg)	Toxicity Class	Hepatotoxicity	Neurotoxicity	Nephrotoxicity	Respiratory toxicity	Cardiotoxicity
Stigmasterol	890	4	Inactive	Active	Inactive	Active	Inactive
gamma.-Sitosterol	890	4	Inactive	Active	Inactive	Active	Inactive

Table 6. Physicochemical properties and drug likeness analysis

Compound name	Mol weight (g/mol)	No. of rotatable bonds	H-bond acceptor	H-bond donor	Molar refractivity	TPSA (Å²)	Consensus LogPo/w	Lipinski rule		Bioavailability score
								Result	Violation	
Stigmasterol	412.69	5	1	1	132.75	20.23	6.98	Yes	1	0.55
gamma.-Sitosterol	414.71	6	1	1	133.23	20.23	7.24	Yes	1	0.55

Fig. 3D & 2D interaction of Stigmasterol with protein PDB: 5VEW

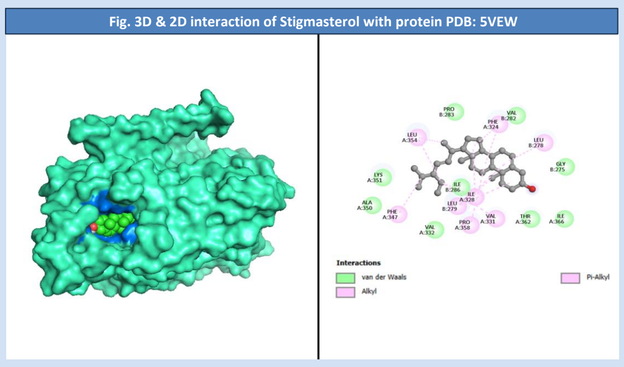


Fig. 3D & 2D interaction of Gamma-Sitosterol with protein PDB:7VSI

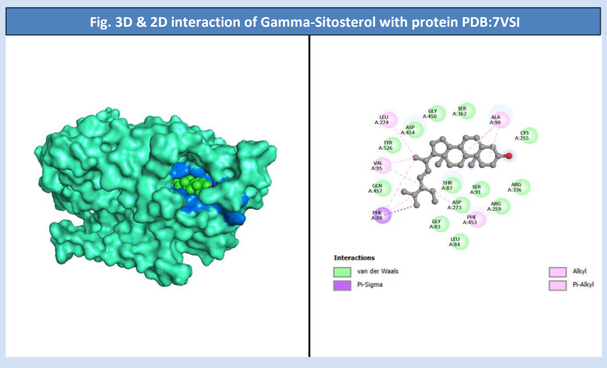


Fig. 3D & 2D interaction of Stigmasterol with protein PDB: 7VOD

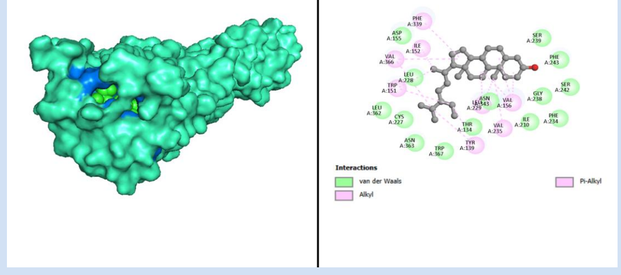
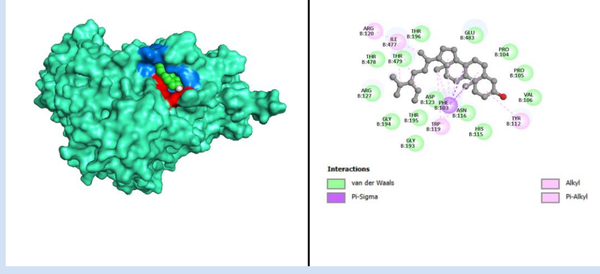


Fig. 3D & 2D interaction of Gamma -Sitosterol with protein PDB: 2V5Z



CONCLUSION

Clitoria ternatea exhibited notable antidiabetic and antidepressant effects, supported by both in silico and in vivo findings. Key phytochemicals, especially stigmasterol and γ-sitosterol, showed strong target binding and favorable pharmacological profiles. Overall, the study suggests that *C. ternatea* may serve as a promising natural source for managing diabetes and related depressive conditions.

FUTURE WORK / REFERENCES

Our future work will involve isolating individual compounds from the extract and evaluating their specific bioactivities

1. Al-Snafi AE. Pharmacological importance of Clitoria ternatea–A review. IOSR journal of Pharmacy. 2016 Mar;6(3):68-83.
2. Islam MA, Mondal SK, Islam S, Akther Shorna MN, Biswas S, Uddin MS, Zaman S, Saleh MA. Antioxidant, cytotoxicity, antimicrobial activity, and in silico analysis of the methanolic leaf and flower extracts of clitoria ternatea. Biochemistry Research International. 2023;2023(1):8847876.