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MOLECULAR DOCKING AND ADMET ANALYSIS OF THE *MUNTINGIA CALABURA* PLANT CONSTITUENT WITH MULTIPLE PHARMACOLOGICAL ACTIVITIES

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ABSTRACT

The identification of novel lead compounds from natural sources is paramount in modern drug discovery. This study employed a dual computational strategy that is in silico molecular docking followed by ADMET analysis to systemically evaluate the therapeutic potential of major phytochemicals isolated from *Muntingia calabura* L. Compounds including key triterpenoids and phenolic acids were screened against 14 established proteins that have been critical targets for seven major therapeutic activities: anti-thrombolytic, anti-oxidant, anti-inflammatory, anti-diabetic, hepatoprotective, COPD, and anti-cancer activities. Binding free energy was used to measure affinity, while drug-likeness rules and predictive toxicity models were used to assess pharmacokinetic property and safety. The docking phase identifies exceptional affinities, notably stigmasterol, b-sitosterol, kaempferol, oleanolic acid, etc., and shows high affinities for respective targets. Critically, the ADMET analysis revealed that the top-performing phytochemicals satisfy the majority of accepted drug-likeness filters and exhibit low-moderate probability for hERG inhibition and AMES mutagenicity. These findings conclude that the traditional use of *Muntingia calabura* positions its potent, druggable constituents as highly promising multi-target lead compounds for pharmacological development.

Key words: *Muntingia calabura* l., Molecular docking, Phytochemicals, Admet analysis, Anti-diabetic, Anti-thrombolytic, anti-inflammatory, Copd, Anti-cancer, Antioxidant, Hepatoprotective.

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INTRODUCTION

Medicinal plants have a valuable source of therapeutic compounds, contributing to the modern drug discovery. The exploration of bioactive phytoconstituents through the computational methods have been increasingly important, particularly with the structure-based drug design tools. Among all tools, molecular docking plays a crucial role by predicting the binding energy and its inhibition constant between small molecules and biological targets. This approach enhances the rapid screening of natural plant constituents and reduce the time consuming and cost with advance experimental drug development.

Muntingia calabura commonly known as the Jamaican cherry plant which is widely distributed in tropical regions. It parts like plant-leaves, fruit and bark have been used as folk medicine for treating ailment such as pain, gastric ulcer and microbial infection and phytochemical investigation of plant have been revealed the presence of diverse bioactive compounds. Many of these compounds exhibit some pharmacological activities The integration of phytochemical knowledge with molecular docking provides a powerful strategy for identifying potential lead compounds from the plant. (Andalia, *et al,*2022). By computing evaluating the interaction between plant derived molecules and specific protein targets, docking studies help to predict the compounds. Such analyses not only validate traditional

medicinal uses of M. calabura but also contribute to the discovery of new drug candidates.

The present study focuses on the molecular docking analysis of selected phytoconstituents from plant against a target protein. The objective is to assess the binding affinities, evaluate key molecular interaction and identify compounds with strongest therapeutic potential. This work provides insight into the molecular basis of the plant's pharmacological effects and supports future experimental validation. (Nguyen *et al,* 2025)

PLANT PROFILE:
***Muntingia calabura* Linn**

Muntingia calabura, commonly known as the Jamaican cherry or "kers," is a medicinal plant widely distributed in tropical regions. Traditionally, various parts of the plant—leaves, fruits, and bark—have been used in folk medicine for treating ailments such as inflammation, pain, gastric ulcers, and microbial infections.

- Kingdom: Plantae
- Clade: Tracheophytes
- Order: Malvales
- Family: Muntingiaceae
- Genus: Muntigia L.
- Species: M.calabura
- Binomial name: Muntigia calabura L.
- Synonyms: Muntingia rosea.

Muntingia calabura is a shrub or tree that quickly grows to between 7.5 and 12 m tall, with spreading branches. The leaves are alternate, distichous, oblong or lanceolate, 4-15 cm long and 1-6 cm wide, with toothed margin and covered in short hairs. The flowers are small (up to 3 cm wide), solitary, or inflorescences of two or three flowers, with five lanceolate sepals, hairy, five obovate white petals, many stamens with yellow anthers and a smooth ovoid ovary. The flowers last only one day, their petals drop in the afternoon. Its fruit is edible berry about 1.5 cm in diameter and with smooth, thin skin, they are green when unripe, turning red when mature. Its pulp is light brown and juicy, with very fine seeds, the pulp tastes like fig. *Muntingia calabura* is native to southern Mexico, the Caribbean, central America, and western south America. It is present in tropical climate in distributed lowland areas from sea level to 1000m of elevation. In south india, it is seen in areas adjacent to the western ghats.

It is planted as a source of timber and fuel. Its soft wood is used for rural construction, while the bark is fibrous and used for making ropes. (Chavez,*et al*,2025) The fruits are edible and, in some cases, sold in market, as they can be eaten raw or processed as jam, leaves can be used for making tea. Also traditional medicinal uses have been reported for the leaves (treating headaches, prostate problem and gastric ulcers), bark (antiseptic), flowers (antiseptic, reducing swelling, antispasmodic) and fruits (respiratory problems, antidiarrheic)

Significance

Muntingia calabura represents an intriguing blend of utility and simplicity. Its capacity to thrive with minimal care makes it an ideal plant for ecological restoration and community green spaces. Its cultural presence, particularly in Southeast Asia and Latin America, marks it as a nostalgic and accessible fruit tree that continues to serve both ecological and social roles.

Phtoconstituents of *Muntingia calabura L.*

1. Gallic acid
2. P-coumaric acid
3. Caffeic acid
4. Ferulic acid
5. Quercetin
6. Rutin
7. Kaempferol
8. Lupenone
9. Oleanolic acid
10. Ursolic acid
11. β – sitosterol
12. Stigmasterol
13. Linoleic acid
14. Lupeol
15. Ellagic acid.

The presence of various phytoconstituents in *Muntingia calabura* L. contributes significantly to the wide range of pharmacological activities. Flavonoids like quercetin, rutin and kaempferol are well known for their potent antioxidant and anti-inflammatory properties, primarily through free radical scavenging and inhibition of pro- inflammatory mediators. Phenolic acids including gallic acid, caffeic acid, ferulic acid and ellagic acid exhibit strong antioxidant, antimicrobial and anticancer activities. Triterpenoids such as oleanolic acid, ursolic acid, lupeol and lupenone have been reported to possess anti-inflammatory, hepatoprotective, antidiabetic and anticancer effects. Additionally, phytosterols like β sitosterol and stigmasterol contribute to cholesterol-lowering and anti-inflammatory activities. Collectively, these bioactive compounds justify the traditional medicinal use of *Muntingia calabura* and highlight its

potential for further pharmacological and in silico drug discovery studies. (Nurhasanah, *et al*, 2023)

METHODS AND METHODOLOGY

Protein Preparation:

The targets of respective pharmacological activities have been derived from the RCSB PDB. Where the crystal structures of targets have been downloaded. The structures are prepared using BIOVIA Discovery Studio 2025 by removing certain atoms and adding charges to it.

Ligand preparation:

The ligands are the phytoconstituents of the *Muntingia calabura* L. plant based on details from the Indian Medicinal Plants, Phytochemistry and Therapeutics (IMPPAT) the respective ligands are downloaded through SMILES from PubChem, CACTUS SMILE TRANSLATOR for PDB conversion.

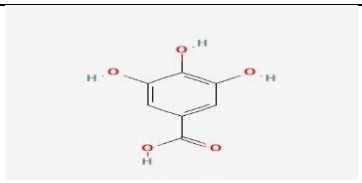
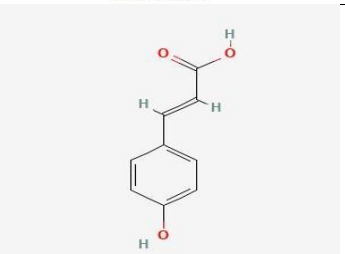
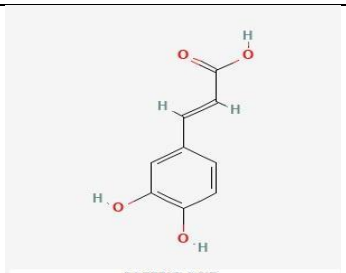
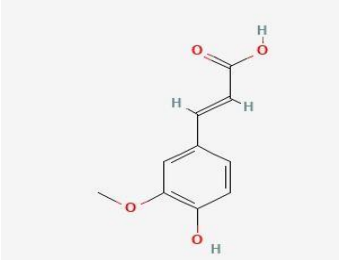
Docking Tools:

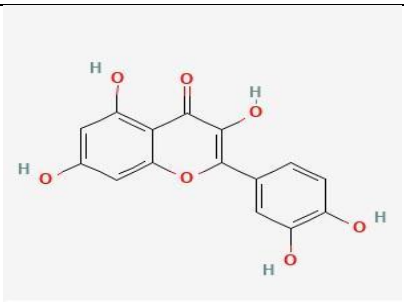
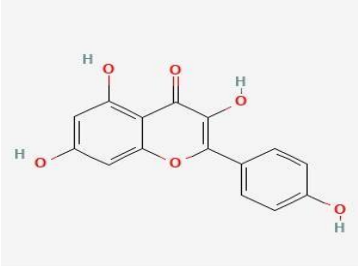
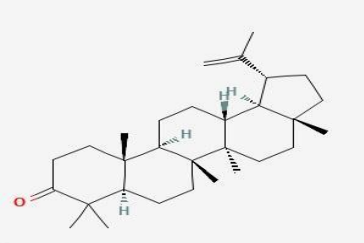
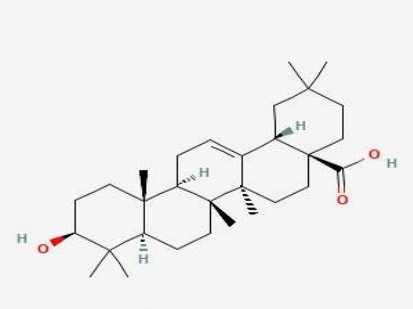
Autodock4, Cygwin, Discovery Studio BIOVIA 2025.

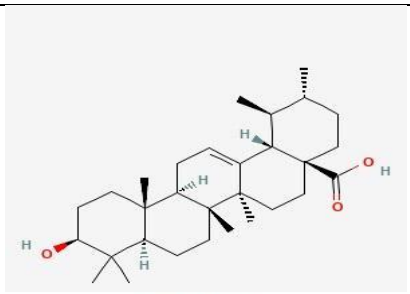
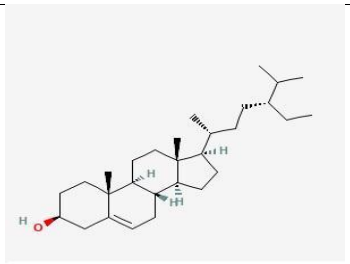
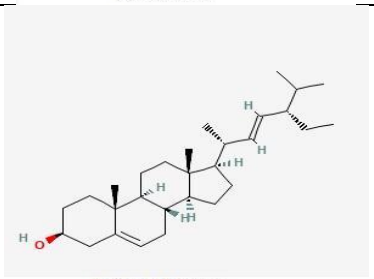
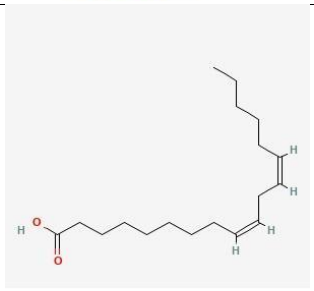
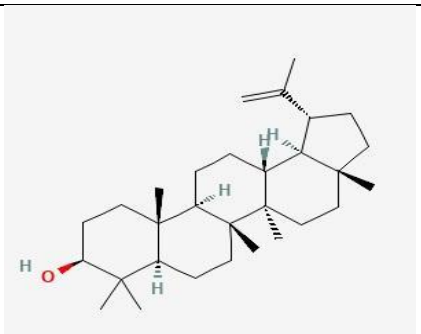
Docking Procedures:

All the targets are downloaded and prepared for docking study using BIOVIA studio, then the ligands are obtained as PDB format using Converter. Therefore, using Autodock4 and Cygwin for the docking scores evaluated. Then the results are evaluated using discovery studio 2025.

Table 1: List of Phytoconstituents

S.NO	PARTS OF PLANS	PHYTOCONSTITUENTS WITH PUBCHEM ID'S	STRUCTURE OF PHYTOCONSTITUENTS
1	LEAF	GALLIC ACID (370)	 GALLIC ACID
2		P-COUMARIC ACID (637542)	 p- COUMARIC ACID
3		CAFFEIC ACID (689043)	 CAFFEIC ACID
4		FERULIC ACID (445858)	 FERULIC ACID

5		QUERCETIN (5280343)	 QUERCETIN
6		RUTIN (5280805)	 RUTIN
7		KAEMPFEROL (5280863)	 KAEMPFEROL
8		LUPENONE (92158)	 LUPENONE
9		OLEANOLIC ACID (10494)	 OLEANOLIC ACID

10		URSOLIC ACID (64945)	 URSOLIC ACID
11	FRUIT	β – SITOSTEROL (222284)	 SITOSTEROL
12		STIGMASTEROL (5280863)	 STIGMASTEROL
13		LINOLEIC ACID (5280440)	 LINOLEIC ACID
14		LUPEOL (259846)	 LUPEOL

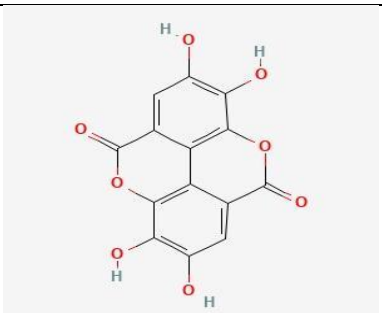
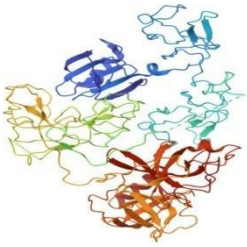
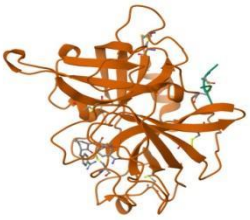
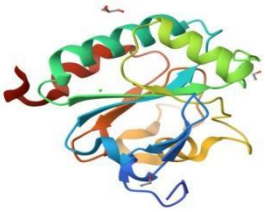
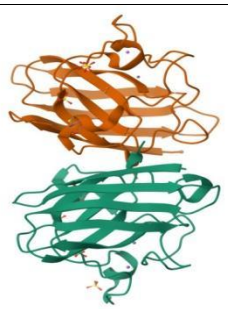
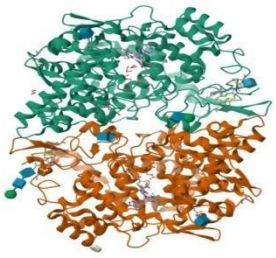
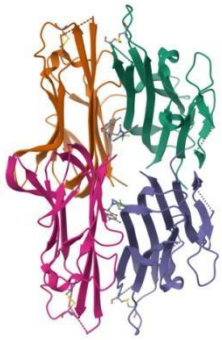
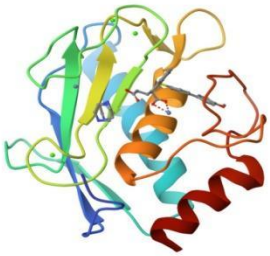
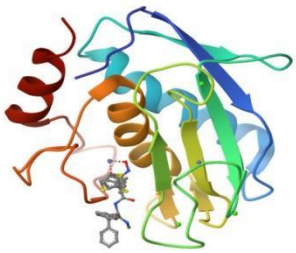
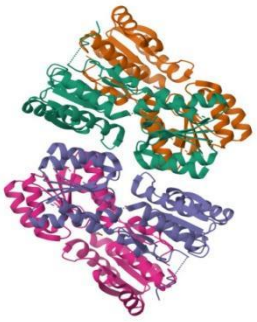
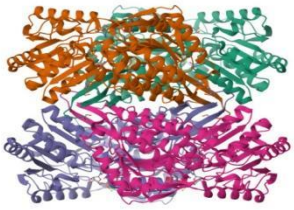
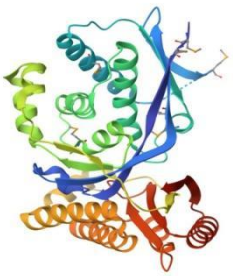
15		ELLAGIC ACID		 ELLAGIC ACID

Table 2: Structures of Targeted Proteins.

S.NO	PHARMACOLOGICAL ACTIVITIES	PDB ID OF TARGETED PROTEIN	STRUCTURE OF TARGETED PROTEIN
1	THROMBOLYTIC ACTIVITY	4DUU	
2	THROMBOLYTIC ACTIVITY	1A5H	
3	ANTI-OXIDANT ACTIVITY	6HN3	

4	ANTI-OXIDANT ACIVITY	2C9V	
5	ANTI-INFLAMMATORY ACTIVTY	5F19	
6	ANTI-INFLAMMATORY ACTIVITY	2AZ5	
7	COPD	6ESM	

8	COPD	1JK3	
9	HEPATOTOXICITY	3E61	
10	HEPATOTOXICITY	1O01	
11	ANTI-CANCER ACTIVITY	1K47	

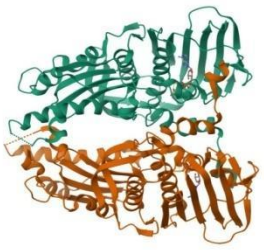
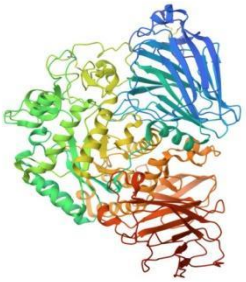
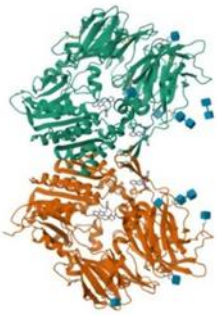
12	ANTI-CANCER ACTIVITY	1ZXM	
13	ANTI-DIABETIC ACTIVITY	3TON	
14	ANTI-DIABETIC ACTIVITY	2ONC	

Table 3: Docking Scores of Thrombolytic Activity

Phytochemicals	Protein: 4DUU		Protein: 1A5H	
	BE(kcal/mol)	IC	BE(kcal/mol)	IC
Gallic acid	-4.84	1.74 µM	-5.09	186.36 µM
P-Coumaric acid	-5.46	99.64 µM	-3.96	1.26 mM
Caffeic acid	-5.08	189.06 µM	-4.19	850.30 µM
Ferulic acid	-5.83	53.92 µM	-7.74	2.11 µM
Quercetin	-6.82	9.97 µM	-4.82	293.91 µM
Rutin	-5.75	60.86 µM	-3.33	3.65 µM
Kaempferol	-6.59	14.72 µM	-5.00	216.32 µM
Lupenone	-8.23	1.30 µM	-7.43	3.66 µM
Oleanolic acid	-8.34	768.84 nM	-7.50	3.17 µM
Ursoilic acid	-7.86	1.74 µM	-7.82	1.85 µM
β Sitosterol	-7.53	3.01 µM	-6.61	14.23 µM
Stigmasterol	-8.01	1.34 µM	-6.88	8.99 µM
Linoleic acid	-4.54	468.35 µM	-3.91	1.36 mM
Lupeol	-7.95	1.50 µM	-7.63	2.55 µM
Ellagic acid	-7.94	1.51 µM	-6.93	8.31 µM

Table 4: Docking Scores of Anti-Oxidant Activity

Phytochemicals	Protein: 6HN3		Protein: 2C9V	
	BE(kcal/mol)	IC	BE(kcal/mol)	IC
Gallic acid	-6.88	8.98 µM	-7.77	2.03 µM
P-Coumaric acid	-7.53	3.05 µM	-7.45	3.43 µM
Caffeic acid	-7.44	1.88 µM	-8.09	1.17 µM
Ferulic acid	-11.90	3.54 µM	-10.31	27.58 nM
Quercetin	-6.39	20.91 µM	-7.24	4.94 µM
Rutin	-5.85	51.54 µM	-10.30	28.26 µM
Kaempferol	-6.03	38.21 µM	-6.48	17.75 µM
Lupenone	-10.27	29.69 nM	-8.92	287.09 µM
Oleanolic acid	-11.89	1.94 nM	-4.93	243.45 µM
Urosilic acid	-12.53	657.59pM	-11.13	7.00 nM
β Sitosterol	-8.68	433.13 nM	-7.33	4.22 µM
Stigmasterol	-9.12	205.59 nM	-7.71	2.22 µM
Linoleic acid	-7.14	5.81 µM	-6.10	34.02 µM
Lupeol	-10.14	38.19 nM	-8.13	1.10 µM
Ellagic acid	-7.18	5.43 µM	-7.17	5.74 µM

Table 5: Docking Scores of Anti- Inflammatory Activity

Phytochemicals	Protein: 5F19		Protein: 2AZ5	
	BE(kcal/mol)	IC	BE(kcal/mol)	IC
Gallic acid	-5.22	148.63 µM	-5.45	101.32 µM
P-Coumaric acid	-6.49	17.56 µM	-5.05	72.47 µM
Caffeic acid	-6.09	34.62 µM	-5.88	48.99 µM
Ferulic acid	-10.29	28.28 nM	-8.11	1.13 µM
Quercetin	-8.60	493.56 nM	-6.22	27.70 µM
Rutin	-8.20	967.88 nM	-4.42	573.83 µM
Kaempferol	-9.59	93.09 nM	-6.10	33.99µM
Lupenone	-10.61	16.80 nM	-7.27	4.69 µM
Oleanolic acid	-10.28	29.23 nM	-8.08	1.19 µM
Urosilic acid	-8.12	1.13 µM	-8.18	1.02 µM
β Sitosterol	-11.89	1.92 nM	-6.58	15.00 µM
Stigmasterol	-13.16	224.67 pM	-6.82	10.09 µM
Linoleic acid	-8.61	489.32 nM	-5.66	71.03 µM
Lupeol	-10.70	14.31 nM	-7.16	5.61 µM
Ellagic acid	-7.81	1.89 µM	-6.09	34.59 µM

Table 6: Docking Scores of COPD

Phytochemicals	Protein: 6ESM		Protein: 1JK3	
	BE(kcal/mol)	IC	BE(kcal/mol)	IC
Gallic acid	-4.70	357.24 µM	-6.53	16.24 µM
P-Coumaric acid	-5.56	83.83 µM	-7.79	1.96 µM
Caffeic acid	-5.53	87.68 µM	-7.75	2.10 µM
Ferulic acid	-1.89	40.92 mM	-0.99	187.52 mM
Quercetin	-8.79	357.75 nM	-10.43	22.58 nM
Rutin	-0.73	538.24 mM	-5.44	102.97 µM
Kaempferol	-9.06	229.39 nM	-10.50	20.20 nM
Lupenone	-3.65	2.12 mM	-5.72	64.08 µM
Oleanolic acid	-2.42	16.82 Mm	-0.92	210.98 mM
Urosilic acid	-5.23	147.00 µM	-5.28	135.90 µM
β Sitosterol	-10.49	20.59 nM	-12.91	346.40 pM
Stigmasterol	-11.56	3.34 nM	-16.28	1.17 pM
Linoleic acid	-6.68	12.80 µM	-9.13	204.55 nM

Lupeol	-4.25	770.49 µM	-4.63	402.20 µM
Ellagic acid	-5.32	126.49 µM	-9.54	100.80 nM

Table 7: Docking Scores of Hepatotoxicity

Phytochemicals	Protein: 3E61		Protein: 1O01	
	BE(kcal/mol)	IC	BE(kcal/mol)	IC
Gallic acid	-5.91	46.81 µM	-4.66	385.95 µM
P-Coumaric acid	-6.87	9.16 µM	-5.09	185.42 µM
Caffeic acid	-6.70	12.25 µM	-5.01	214.48 µM
Ferulic acid	-4.87	269.34 µM	-8.32	792.22 nM
Quercetin	-8.14	1.08 µM	-8.14	1.08 µM
Rutin	-8.87	316.88 nM	-5.04	203.13 µM
Kaempferol	-7.86	229.39 nM	-7.68	2.33 nM
Lupenone	-10.28	29.18 nM	-9.49	110.97 nM
Oleanolic acid	-4.86	275.34 µM	-8.29	839.69 nM
Urosilic acid	-5.92	46.16 µM	-8.24	905.99 nM
β Sitosterol	-11.91	1.42 nM	-9.93	52.76 nM
Stigmasterol	-12.07	467.95 nM	-9.86	58.79 nM
Linoleic acid	-8.64	56.68 nM	-5.94	44.03 µM
Lupeol	-9.94	1.67 µM	-9.86	59.24 nM
Ellagic acid	-11.97	11.63 nM	-6.11	33.37 nM

Table 8: Docking Scores of Anti-Cancer Activity

Phytochemicals	Protein: 1K47		Protein: 1ZXM	
	BE(kcal/mol)	IC	BE(kcal/mol)	IC
Gallic acid	-7.19	5.39 µM	-5.87	49.91 µM
P-Coumaric acid	-6.97	7.81 µM	-6.69	7.86 µM
Caffeic acid	-9.96	50.18 µM	-6.98	7.69 µM
Ferulic acid	-9.95	50.69 µM	-9.68	80..04 nM
Quercetin	-5.86	48.32 µM	-7.02	7.19 µM
Rutin	-4.84	281.20 µM	-4.48	520.29 µM
Kaempferol	-7.30	4.45 µM	-6.42	19.59 µM
Lupenone	-8.78	366.34 nM	-8.37	732.48 Nm
Oleanolic acid	-9.94	5.1.02 nM	-9.71	76.05 Nm
Urosilic acid	-10.15	36.88 nM	-9.64	86.47 nM
β Sitosterol	-7.03	6.98 µM	-7.70	2..27µM
Stigmasterol	-7.06	6.64 µM	-7.82	1.84 µM
Linoleic acid	-6.63	13.82 µM	-5.73	62.80 µM
Lupeol	-8.94	278.44 nM	-8.26	886.00 Nm
Ellagic acid	-6.97	7.77 µM	-6.81	10.11 µM

Table 9: Docking Scores of Anti-Diabetic Activity

Phytochemicals	Protein: 3TON		Protein: 20NC	
	BE(kcal/mol)	IC	BE(kcal/mol)	IC
Gallic acid	-3.87	1.45 mM	-6.76	11.03 µM
P-Coumaric acid	-4.41	585.46 µM	-4.76	322.84 µM
Caffeic acid	-4.30	708.45 µM	-4.94	238.12 µM
Ferulic acid	-6.86	9.29 µM	-7.77	2.00 µM
Quercetin	-5.95	43.16 µM	-6.47	18.18 µM
Rutin	-4.36	635.43 µM	-4.47	526.47 µM
Kaempferol	-5.99	40.68 µM	-5.99	40.83 µM
Lupenone	-7.82	1.87 µM	-9.11	210.74 nM
Oleanolic acid	-6.81	10.28 µM	-7.78	1.99 µM
Urosilic acid	-6.96	7.97 µM	-8.27	869.20 nM

β Sitosterol	-6.86	9.41 µM	-8.02	1.32 µM
Stigmasterol	-7.23	5.01 µM	-9.22	175.00 nM
Linoleic acid	-2.92	7.23 µM	-4.53	478.48 µM
Lupeol	-7.71	2.22 µM	-8.85	324.27 nM
Ellagic acid	-6.15	31.08 µM	-6.70	12.28 µM

Table 10: SwissADME Analysis of *Muntingia calabura* plant phytoconstituents

Phyto-Constituents	MW g/mol	HBA	HBD	Bio Availabity Score	GI Absorption	BBB	LIPINSKI RULE
Gallic acid	170.12	5	4	0.56	High	No	Yes
p-coumaric acid	164.16	3	2	0.85	High	Yes	Yes
Caffeic acid	180.16	4	3	0.56	High	No	Yes
Ferulic acid	194.18	4	2	0.85	High	Yes	Yes
Quercetin	302.24	7	5	0.55	High	No	Yes
Rutin	610.52	16	10	0.17	Low	No	No
Kaempferol	286.24	6	4	0.55	High	No	Yes
Lupenone	424.70	1	0	0.55	Low	No	Yes
Oleanolic acid	456.70	3	2	0.85	Low	No	Yes
Ursolic acid	456.70	3	2	0.85	Low	No	Yes
b- sitosterol	414.71	1	1	0.55	Low	No	Yes
Stigmasterol	412.69	1	1	0.55	Low	No	Yes
Linoleic acid	280.45	2	1	0.17	Low	No	No
Lupeol	426.72	1	1	0.55	Low	No	Yes
Ellagic acid	302.19	8	4	0.55	High	No	Yes

Table 11: pkCSM for the excretion and toxicity studies

Phyto-Constituents	Total Clearance ml/min/kg	Ames Toxicity	Max-Tolerated Dose(Human) mg/kg/day	Hepato-Toxicity	Skin Sensitization	LD50 Mol/kg
Gallic acid	0.518	No	0.7	No	No	2.218
p-coumaric acid	0.662	No	1.111	No	No	2.155
Caffeic acid	0.508	No	1.145	No	No	2.383
Ferulic acid	0.623	No	1.082	No	No	2.282
Quercetin	0.407	No	0.499	No	No	2.471
Rutin	-0.369	No	0.452	No	No	2.491
Kaempferol	0.477	No	0.531	No	No	2.449
Lupenone	0.102	No	0.008	No	No	2.556
Oleanolic acid	-0.081	No	0.094	Yes	No	2.196
Ursolic acid	0.083	No	0.199	Yes	No	2.346
b- sitosterol	0.628	No	-0.621	No	No	2.552
Stigmasterol	0.618	No	-0.664	No	No	2.54
Linoleic acid	1.936	No	-0.827	Yes	Yes	1.429
Lupeol	0.153	No	-0.502	No	No	2.563
Ellagic acid	0.537	No	0.476	No	No	2.399

Figure 2 Docking visual of thrombolytic targets

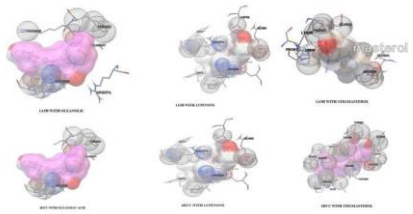


Figure 3 docking visuals of Anti- oxidant targets

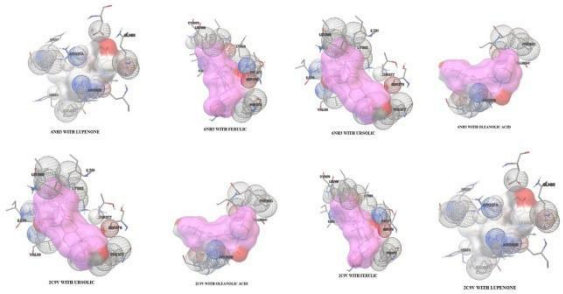


Figure 4 Docking visuals of Anti- inflammatory Targets

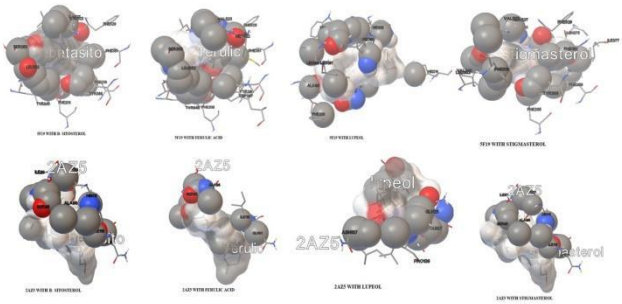


Figure 5 Docking visuals of COPD targets

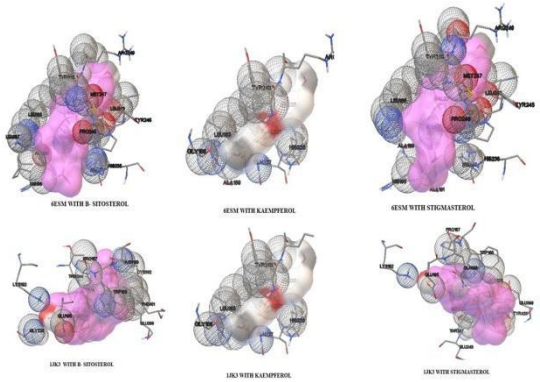


Figure 6 Docking visuals of Hepatotoxicity Targets

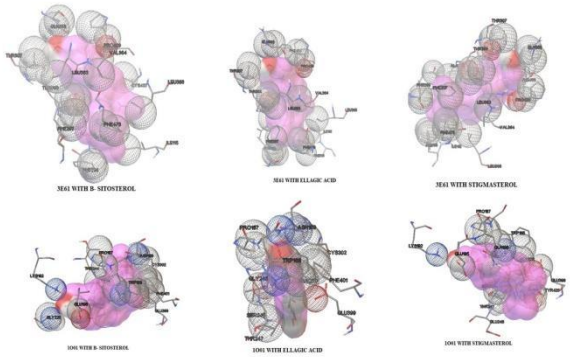
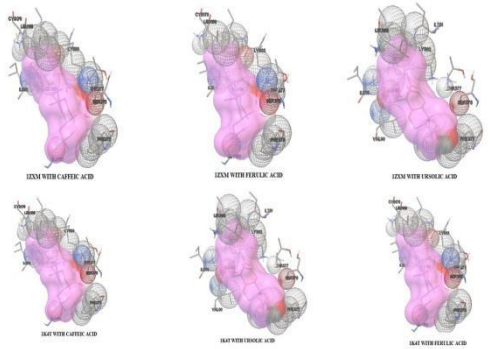


Figure 7 Docking visuals of Anti- cancer Targets



RESULTS AND DISCUSSION

DOCKING SCORES:

All the targets of respective activities are tested and evaluated using the binding free energy and inhibition constant and determines the potential of the ligands towards the target.(Prayogi, *et al*, 2025) general rule in the docking study that is,

More negative binding energy = better binding affinity

Lower inhibition constant = stronger inhibition

For Thrombolytic activity:

Muntingia calabura L., is evaluated for its thrombolytic property and effectiveness towards the thrombolytic activity. For this study, the selected targets were PDB 4DUU & PDB 1A5H.

From the above docking scores of 15 different phytoconstituents with two different mechanism possessing targets it gives that this plant constituents have a potential thrombolytic activity, based on the general rule some phytoconstituents has a good result based on the

binding energy. They are oleanolic acid, lupenone and stigmasterol with binding affinity of -8.34 kcal/mol, -8.23 kcal/mol, -8.01 kcal/mol with 4DUU and -7.50 kcal/mol, 7.42 kcal/mol, -6.88 kcal/mol with 1A5H targets respectively. (Mildawati, *et al*, 2025**)**

Antioxidant Activity:

It is evaluated for its anti-oxidant property and effectiveness towards the antioxidant activity. For this study the selected targets were PDB 6HN3 & PDB 2C9V. (Hamoud Alseagh, *et al*,2025)

From the above docking scores of 15 different phytoconstituents with two different mechanism possessing targets it gives that this plant constituents have a potential antioxidant activity, based on the general rule some phytoconstituents has a good result based on the binding energy. They are ursolic acid, oleanolic acid, ferulic acid and lupenone with binding affinity of -12.53 kcal/mol, -11.89 kcal/mol, -11.90 kcal/mol, -10.27 kcal/mol with 6HN3 and -11.13 kcal/mol, -4.93 kcal/mol, -10.31 kcal/mol, -8.92 kcal/mol with 2C9V targets respectively. And their inhibition constant also gives a good result against the respective targets. (Rajesh, *et al,*2014)

For Anti-inflammatory Activity:

Evaluation of *Muntingia calabura* L., has been done against the inflammatory targets. They are 5F19 & 2AZ5.

From the above docking scores of 15 different phytoconstituents with two different mechanism possessing targets it gives that this plant constituents have a potential anti-inflammatory activity, based on the general rule some phytoconstituents has a good result based on the binding energy. (Nurhasanah, *et al*,2024) They are stigmasterol, beta-sitosterol, ferulic acid and lupeol with binding affinity of -13.16 kcal/mol, -11.89 kcal/mol, -10.29 kcal/mol, -10.70 kcal/mol with 5F19 and -6.82 kcal/mol, -6.58 kcal/mol, -8.11 kcal/mol, -7.16 kcal/mol with 2AZ5 targets respectively. And their inhibition constant also gives a good result against the respective targets. (Rezeki, *et al*,2023)

For COPD:

The evaluation of *Muntingia calabura* L., has been done against the COPD targets. They are 6ESM & 1JK3.

From the above docking scores of 15 different phytoconstituents with two different mechanism possessing targets it gives that this plant constituents have a potential COPD activity, based on the general rule some phytoconstituents has a good result based on the binding energy. (Shawky, *et al*,2020) They are stigmasterol, beta-sitosterol and kaempferol with binding affinity of -11.56 kcal/mol, -10.49 kcal/mol, -9.06 kcal/mol with 6ESM and -16.28 kcal/mol, -12.91 kcal/mol, -10.50 kcal/mol with 1JK3 targets respectively. And their inhibition constant also gives a good result against the respective targets. (Lakshmi Sundaram R, *et al,*2025)

For hepatotoxicity:

The evaluation of *Muntingia calabura* L., has been done against the hepatotoxicity targets. They are 3E61& 1O01.

From the above docking scores of 15 different phytoconstituents with two different mechanism possessing targets it gives that this plant constituents have a potential hepatotoxicity activity, based on the general rule some phytoconstituents has a good result based on the binding energy. They are stigmasterol, beta-sitosterol and ellagic acid with binding affinity of -12.07 kcal/mol, -11.91 kcal/mol, -11.97 kcal/mol with 3E61 and -9.86 kcal/mol, -9.93 kcal/mol, -6.11 kcal/mol with 1O01 targets respectively. (Bandeira, *et al,*2012) And their inhibition constant also gives a good result against the respective targets.

For Anti- Cancer activity:

The evaluation of *Muntingia calabura* L., has been done against the anti-cancer targets. They are 1K47& 1ZXM.

From the above docking scores of 15 different phytoconstituents with two different mechanism possessing targets it gives that this plant constituents have a potential anti-cancer activity, based on the general rule some phytoconstituents has a good result based on the binding energy. (Chaudhari, *et al*,2020) They are ursoilic acid caffeic acid and Ferulic acid with binding affinity of -10.15 kcal/mol, -9.96 kcal/mol, -9.95 kcal/mol with 1K47 and -9.64 kcal/mol, -6.98 kcal/mol, -9.68 kcal/mol with 1ZXM targets respectively. And their inhibition constant also gives a good result against the respective targets. (A., Mohsen, *et al,*2021)

For Anti- Diabetic activity:

The evaluation of *Muntingia calabura* L., has been done against the anti-diabetic targets. They are 3TON& 20NC.

From the above docking scores of 15 different phytoconstituents with two different mechanism possessing targets it gives that this plant constituents have a potential anti-inflammatory activity, based on the general rule some phytoconstituents has a good result based on the binding energy. They are stigmasterol, beta-sitosterol and lupeol with binding affinity of -7.23 kcal/mol, -6.86 kcal/mol, -7.71 kcal/mol with 3TON and -9.22 kcal/mol, -8.02 kcal/mol, -8.55 kcal/mol with 20NC targets respectively. And their inhibition constant also gives a good result against the respective targets

Note:

mM = 10^{-3} m (largest)

µM = 10^{-6} m

pM = 10^{-12} m (smallest)

BE = binding energy

IC = inhibition constant

Admet Analysis of *Muntingia calabura* Linn

For the analysis of absorption, distribution, metabolism, excretion and toxicity of a plant phytoconstituents it was first obtained from the IMPPAT database then its SMILES are taken into the SwissADME analyser for absorption, distribution, metabolism and for excretion and toxicity study the pkCSM software is used. Based on this we analyse the ADMET profiles of phytoconstituents with molecular weight(MW), hydrogen bond acceptor (HBA), hydrogen bond donor (HBD), bioavailability score, GI absorption, BBB permeation, Lipinski rule, total clearance, AMES toxicity and LD50 etc. (Koirala, *et al*,2017)

The phytoconstituents of *Muntingia calabura* exhibit diverse ADMET profile. Phenolic acids like gallic acid, caffeic acid, p- coumaric acid and ferulic acid shows high GI absorption with moderate bioavailability ranges from 0.55 – 0.85, making it as promising one for oral administration. Among these the p-coumaric and ferulic acid are also predicted to cross the blood- brain barrier, suggesting potential CNS activity. Flavonoids like quercetin, kaempferol and ellagic acid shows moderate absorption and bioavailability but do not cross BBB. Larger molecule including rutin, triterpenoids shows low GI absorption and variable bioavailability, suggesting that alternate delivery route is required for therapeutic effectiveness. (Kontoyianni, *et al,*2003)

Toxicity prediction indicates that most of the compounds are non-mutagenic (AMES negative) with high LD50 values, suggesting low acute toxicity. Certain triterpenoids exhibit potential hepatotoxicity, highlights the need of careful dose management and its LD50 indicates the moderate to low toxicity for majority of the componuds Overall the phytochemical of *Muntingia calabura* demonstrates a favorable safety profile with promising oral bioavailability for several small phenolic compounds. (Setyaningsih, *et al,*2019)

CONCLUSION

The present study works on the dual computational method that is in silico molecular docking followed by ADMET analysis to evaluate the therapeutic evaluation of major phytoconstituents of *Muntingia calabura* L. For this several softwares are used to predict the drug potency. From this study that the triterpenoids and phenolic acid have been shown good drug-likeness and predictive toxicity against the critical targets of seven major pharmacological activities, which shown that these compounds have some potential activity with their pharmacological targets. And their toxicity level are also mild- moderate with an evidence of toxicity studies, for this total 14 targets are used against 15 phytoconstituents and their findings shown that it can be a potential drug-likeness in future. These conclude that the traditional use of *Muntingia calabura* is potent and druggable constituents as highly promising multi-target lead compounds for pharmacological development with future in vitro and in vivo methods.

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