e-ISSN: 2249 – 7781
Print ISSN: 2249 – 779X

International Journal of Pharmaceutical Research & Analysis
www.ijpra.com

Review Article

MOLECULAR DOCKING AND ADMET ANALYSIS OF THE ABUTILON INDICUM PLANT CONSTITUENT WITH MULTIPLE PHARMACOLOGICAL ACTIVITIES

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ABSTRACT

Abutilon indicum (L.), a medicinal plant of the Malvaceae family, has long been valued in traditional medicine for its diverse pharmacological activities, including anti-inflammatory, antimicrobial, antioxidant, antidiabetic, and hepatoprotective effects. Despite its ethnomedicinal importance, the molecular mechanisms underlying these therapeutic properties remain insufficiently explored. In this study, molecular docking was performed to evaluate the binding affinities of major phytoconstituents of Abutilon indicum against selected protein targets associated with inflammation, microbial resistance, oxidative stress, and cancer progression. Docking simulations revealed that flavonoids, alkaloids, and phenolic compounds exhibited strong interactions, suggesting multi-target pharmacological potential.To complement these findings, ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) analysis was conducted to assess pharmacokinetic behaviour and drug-likeness. Most compounds complied with Lipinski's rule of five, demonstrated favourable oral bioavailability, and showed low predicted toxicity, indicating their suitability as lead molecules for drug development. The integration of docking and ADMET profiling provides a comprehensive in silico framework for identifying promising bioactive compounds from Abutilon indicum. These results validate its traditional use and highlight its potential role in modern drug discovery, warranting further experimental and clinical investigations.

Keywords: Abutilon indicum; molecular docking; ADMET analysis; phytoconstituents; pharmacological activities; drug-likeness; Lipinski's rule; in silico drug discovery; multi-target therapy.

INTRODUCTION

Medicinal plants have long served as a cornerstone of traditional healthcare systems, offering bioactive compounds with diverse therapeutic potential. In recent years, computational approaches such as molecular docking and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) analysis have emerged as powerful tools to predict drug-target interactions and pharmacokinetic behaviour of phytoconstituents. These in silico methods accelerate drug discovery by identifying promising lead molecules prior to experimental validation.Abutilon indicum (L.), commonly known as Indian mallow, is a medicinal plant widely distributed across tropical and subtropical regions. It has been traditionally employed in Ayurveda, Siddha, and Unani systems of medicine for the treatment of ailments such as inflammation, diabetes, jaundice, ulcers, and microbial infections. Modern pharmacological studies have confirmed its anti-inflammatory, antimicrobial, antioxidant, hepatoprotective, antidiabetic, and anticancer properties, underscoring its multi-target therapeutic relevance.Despite extensive ethnomedicinal use, systematic computational evaluation of Abutilon indicum phytoconstituents remains limited. Molecular docking can provide insights into the binding affinities of its bioactive compounds with key protein targets, while ADMET profiling ensures their suitability as drug candidates. This integrated approach not only validates traditional knowledge but also facilitates the

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Aakash N

identification of novel therapeutic leads for modern drug development.

Plant Profile

Figure 1: Abutilon Indicum

Scientific Classification

- Family: Malvaceae
- Genus: *Abutilon*
- Species: *Abutilon indicum* (L.) Sweet

- **Common Names**
  - Indian mallow, Atibala (Ayurveda), Kanghi, Thuthi (Tamil) and Country mallow.
- **Morphology**
  - A perennial shrub, 1–2 meters in height.

Leaves: Heart-shaped, velvety, with serrated margins.

- Flowers: Yellow, solitary, axillary, resembling small hibiscus.
- Fruits: Capsule with multiple seeds.

- **Distribution**
  - Widely found in tropical Asia, Africa, and the Indian subcontinent, especially in wastelands and roadsides.

Pharmacological Activities

- Anti-inflammatory, antimicrobial, antioxidant, hepatoprotective, antidiabetic, analgesic, and anticancer effects have been reported in experimental studies.

Phytoconstituen

- Quercetin
- Luteolin
- Kaempferol
- Apigenin
- Naringenin
- Rutin
- Catechin
- Gallic acid
- Caffeic acid
- Ferulic acid
- β-Sitosterol
- Stigmasterol
- Lupeol
- β -Amyrin
- Squalene.

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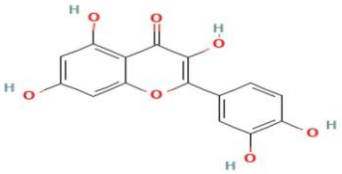
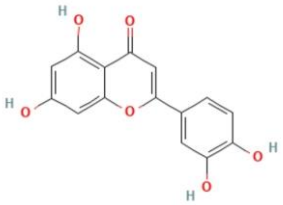
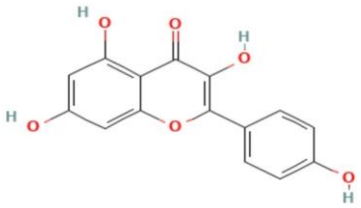
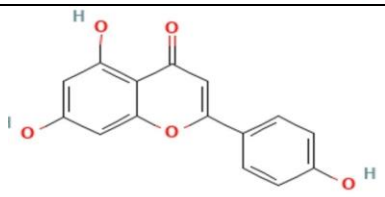
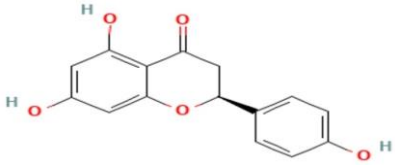
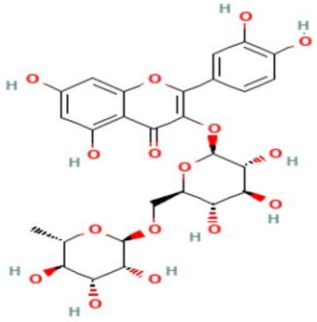
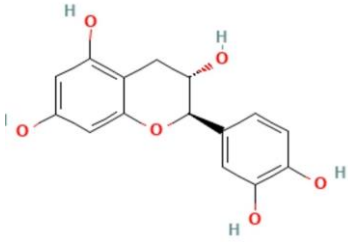
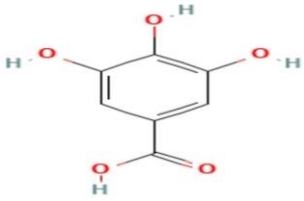
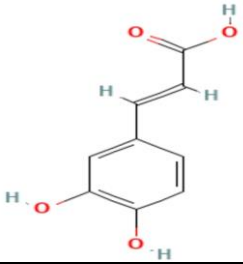
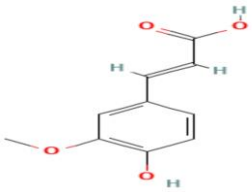
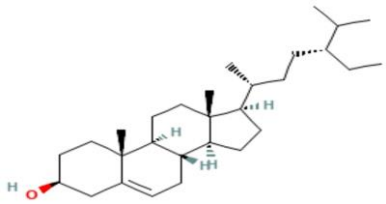
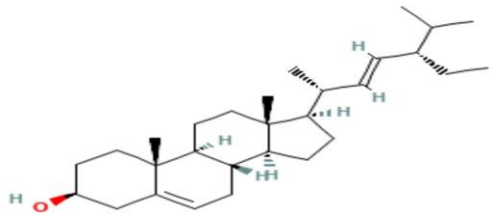
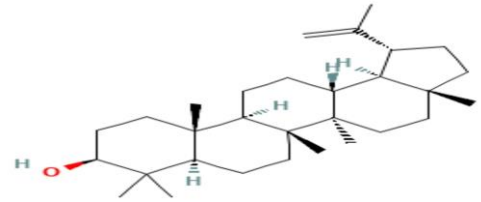
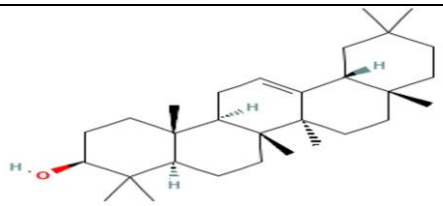
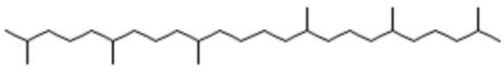
1.	**Quercetin (5280343)**	
2.	**Luteolin (5280445)**	

3.	**Kaempferol (5280863)**	
4.	**Apigenin (5280443)**	
5.	**Naringenin (932)**	
6.	**Rutin (5280805)**	
7.	**Catechin (9064)**	
8.	**Gallic acid (370)**	
9.	**Caffeic acid (689043)**	

10.	**Ferulic acid (445858)**	
11.	**β sitosterol (222284)**	
12.	**Stigmasterol (5280794)**	
13.	**Lupeol (259846)**	
14.	**β Amyrin (73170)**	
15.	**Squalene (638072)**	

MATERIALS AND METHODOLOGY

Protein Preparation

- **Protein Source:** The three-dimensional structure of the target protein was retrieved from the **Protein Data Bank (PDB)** in .pdb format.
- **Preprocessing:**
  - Removal of water molecules, heteroatoms, and co-crystallized ligands.
  - Addition of hydrogen atoms to stabilize the structure.
  - Assignment of correct bond orders and protonation states.

Ligand Preparation

- **Ligand Source:** Ligand structures were obtained from databases such as **PubChem**.
- **Optimization:**
  - Conversion to 3D structures using software like BIOVIA
  - Addition of hydrogen atoms and assignment of charges.
  - Energy minimization using molecular mechanics force fields.
- **File Format:** Ligands were saved pdbqt format for docking compatibility.

Docking Tools

- **Software Used:**
  - **AutoDock Vina** for docking simulations.
  - **Discovery Studio Visualizer** for visualization of protein-ligand interactions.

Docking Procedures

- **Grid Box Generation:**
  - Active site coordinates were defined based on known binding pockets or co-crystallized ligands.
  - A grid box was set to encompass the binding site region.
- **Docking Simulation:**
  - Ligands were docked into the protein binding site using AutoDock Vina.
  - Multiple conformations were generated and ranked based on binding affinity scores.
- **Analysis of Results:**
  - Binding energies (kcal/mol) were recorded.
  - Hydrogen bonds, hydrophobic interactions, and π–π stacking were analyzed.
  - Best docking poses were visualized and compared with reference ligands.

RESULT 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.general rule in the docking study that is,

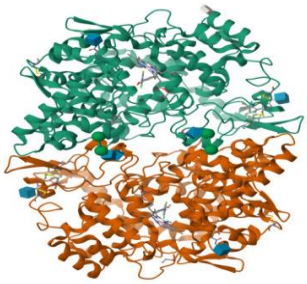
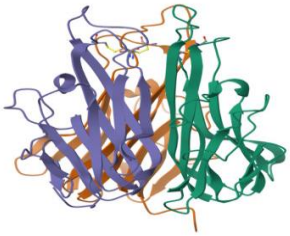
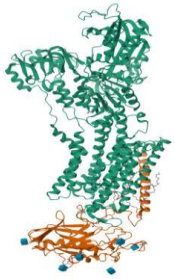
More negative binding energy = better binding

Lower inhibition constant = stronger inhibition.

For Anti-inflammatory Activity:

Abutilon Indicum is evaluated for its anti-inflammatory property and effectiveness towards its anti-inflammatory activity. For this study, the selected targets were PBD 51KQ & PBD 1TNF.

Table 2: Structures of Targeted Proteins

S.NO.	Pharmagological Activities	Targeted Protein with PBD ID	Structure of Targeted Protein
1.	**ANTI-INFLAMMATORY ACTIVITY**	**COX-2 (51KQ)**	
		TNF-α (1TNF)	
2.	**ANTI-ULCER ACTIVITY**	**H+K+ ATPase (6JXJ)**	

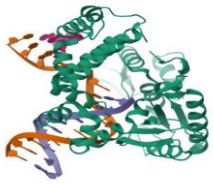
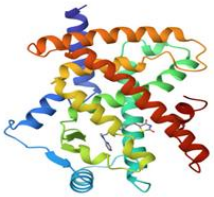
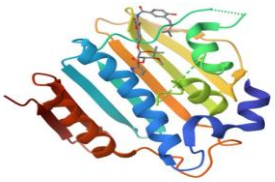
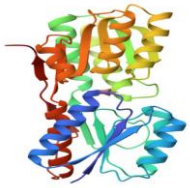
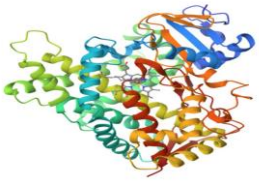
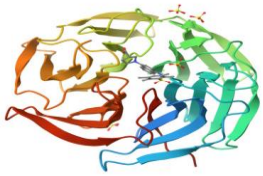
		H2(5U8H)	
3.	**ANTI-DIABETIC ACTIVITY**	**PPAR-γ (2PRG)**	
		α-GLUCOSIDE (3A4A)	
4.	**ANTI-MICROBIAL ACTIVITY**	**DNA GYRASE (1KZN)**	
		DHFR (1DRI)	
5.	**HEPOTOPROTECTIVE ACTIVITY**	**CYPZE1 (3LC4)**	
		KEAPINRF2 (5CGJ)	

Table 3: Docking Scores of Anti-Inflammatory Activity

Phytochemicals	Protein:51KQ		Protein:1TNF	
	BE(kcal/mol)	IC	BE(kcal/mol)	IC
Quercetin	-8.58	510.27 nm	-5.96	42.58 µm
Luteolin	-8.83	335.81 nm	-7.61	2.63 µm
kaempferol	-8.32	797.12 nm	-6.77	10.85 µm
Apigenin	-8.46	633.66 nm	-6.60	14.56 µm
Naringenin	-8.39	711.29 nm	-7.52	3.06 µm
Rutin	-8.16	1.04 µm	-0.35	550.81 MM
Catechin	-5.80	56.34 µm	-6.56	15.62 µm
Gallic acid	-8.24	909.25 nm	-6.26	26.66 µm
Caffeic acid	-6.78	10.68 µm	-5.81	55.17 µm
Ferulic acid	-7.15	5.73 µm	-5.96	42.87 µm
β - sitosterol	-11.28	5.41 nm	+20.54	15.62 µm
Stigmasterol	-11.34	4.89 nm	+11.65	15.62 µm
Lupeol	-10.21	32.61 nm	-8.56	527.32 nm
β - Amyrin	-10.5	20.01 nm	+130.79	3.06 µm
Squalene	-8.74	390.20 nm	+27.18	3.06 µm

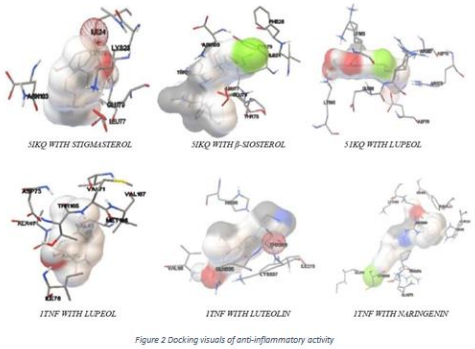


Figure 2 Docking visuals of anti-inflammatory activity

From the above docking scores of 15 phytoconstituents with two different mechanism possessing targets it gives that this plant constituents have a potential anti-inflammatory activity, based on the general rule of some phytoconstituents has a good result based on the binding energy. They are stigmasterol, β-sitosterol and lupeol with the binding affinity of -11.34 kcal/mol, -11.28 kcal/mol and -10.50 kcal/mol with 5IKQ.They are Lupeol, Luteolin, Naringenin with the binding affinity of -8.56 kcal/mol, -7.61 kcal/mol and -7.52 kcal/mol with 1TNF. And the inhibition constant also good result against the respective targets.

FOR ANTI-ULCER ACTIVITY:

For evaluation of ABUTILON INDICUM has against the anti-ulcer targets. They are 6JXJ and 5U8H.

Table 4: Docking Scores of Antis–Ulcer Activity

Phytochemicals	**Protein:6JXJ**		**Protein:5U8H**	
	BE (kcal/mol)	**IC**	**BE (kcal/mol)**	**IC**
Quercetin	-5.56	84.21µm	-5.91	46.89µm
Luteolin	-5.93	44.64µm	-6.27	25.42µm
Kaempferol	-5.95	43.71µm	-6.08	35.20µm
Apigenin	-6.60	14.56µm	-6.07	35.51µm
Naringenin	-5.80	50.85µm	-5.86	50.85µm
Rutin	-3.91	1.36mm	-3.02	6.16mm
Catechin	-5.77	58.99µm	-5.77	58.99µm
Gallic acid	-3.76	1.76mm	-4.35	650.36µm
Caffeic acid	-5.36	117.86µm	-5.19	157.07µm
Ferulic acid	-5.27	136.11µm	-5.42	106.01µm
β- sitosterol	-8.59	508.61nm	-8.50	589.22nm

Stigmasterol	-9.51	107.56nm	-8.60	493.05nm
Lupeol	-10.74	36.92nm	-8.56	527.92nm
β - Amyrin	-9.42	124.17nm	-8.43	664.98nm
Squalene	-5.45	101.96µm	-5.46	99.45µm

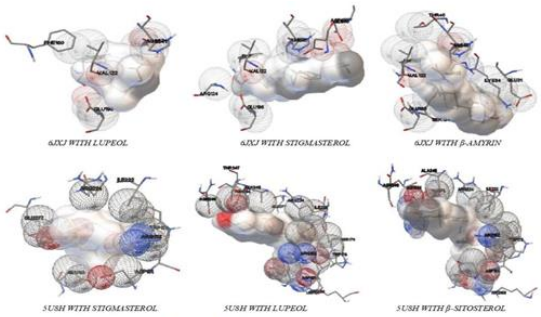


Figure 3 Docking visuals of Anti-ulcer activity

From the above docking scores of 15 different phytoconstituents with two different mechanism possessing target its gives that this phytoconstituents have a potential anti-ulcer activity, based on the general rule of phytoconstituents has a good result based on the binding energy. They are Lupeol, Stigmasterol and β-Amyrin with binding affinity of -10.74 kcal/mol, -9.51 kcal/mol and -9.42 kcal/mol with 6JXJ. They are also Stigmasterol, Lupeol and β-sitosterol with binding affinity of -8.60 kcal/mol , -8.50 kcal/mol and -8.43 kcal/mol with 5U8H. And their inhibition constant also good results against the respective targets.

FOR ANTI-DIABETIC ACTIVITY: The evaluation of *Abutilon Indicum* has been done against the *Anti-Microbial Targets*. They are 2PRG and 3A4A.

Table 5: Docking Scores of Anti-Diabeticactivity

PHYTOCHEMICALS	Protein: 2PRG		Protein:3A4A	
	BE (kcal/mol)	IC	BE (kcal/mol)	IC
Quercetin	-6.19	28.91µm	-7.18	5.49µm
Luteolin	-7.52	3.07µm	-7.92	1.56µm
kaempferol	-5.99	40.61µm	-6.98	7.60µm
Apigenin	-7.48	3.30µm	-7.87	1.69µm
Naringenin	-7.86	1.74µm	-7.93	1.53µm
Rutin	-5.44	102.93µm	-5.57	82.20µm
Catechin	-6.79	10.49µm	-7.86	1.74µm
Gallic acid	-5.29	132.86µm	-2.54	13.80mm
Caffeic acid	-5.23	145.78µm	-4.60	425.51µm
Ferulic acid	-4.94	238.95µm	-4.41	581.23µm
β - sitosterol	-7.35	4.12µm	-11.26	5.60nm
Stigmasterol	-8.68	436.45µm	-11.14	6.83nm
Lupeol	-8.09	1.17µm	-9.04	234.95nm
β-Amyrin	-7.66	2.42µm	-8.78	366.82nm
Squalene	-4.53	479.99µm	-7.99	1.40µm

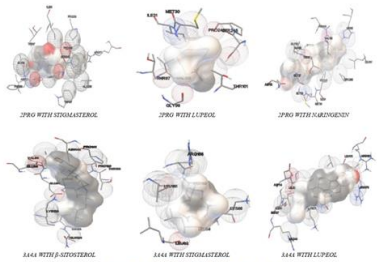


Figure 4 Docking visuals for anti-diabetic activity

From the above docking scores 15 phytoconstituents with two different proteins and that gives the plant phytoconstituents have a good Anti-diabetic activity, based on the general rule the phytoconstituents have good anti-diabetic activity. They are Stigmasterol, Lupeol and Naringenin with their binding energy is -8.68 kcal/mol, -8.09 kcal/mol and -7.86 kcal/mol with 2PRG. And they are β-sitosterol, Stigmasterol and Lupeol and their binding energy are -11.26 kcal/mol, -11.14 kcal/mol and -9.04 kcal/mol with 3A4A targets respectively. And their inhibition constant also gives a good result against the respective targets.

FOR ANTI-MICROBIAL ACTIVITY: The evaluation of *Abutilon Indicum* has been done against the *Anti-Microbial Targets*. They are 1KZN and 1AI9.

Table 6: Docking Scores of Anti-Microbial Activity

PHYTOCHEMICAL	Protein:1KZN		Protein:1AI9	
	BE (kcal/mol)	IC	BE (kcal/mol)	IC
Quercetin	-7.38	3.92µm	-8.12	1.45µm
Luteolin	-7.15	5.72µm	-8.18	1.02µm
kaempferol	-7.36	4.00µm	-7.85	1.75µm
Apigenin	-7.77	2.01µm	-7.79	1.92µm
Naringenin	-7.82	1.85µm	-8.21	957.52µm
Rutin	-4.24	773.89µm	-5.83	53.71µm
Catechin	-7.45	3.47µm	-7.92	2.05µm
Gallic acid	-3.43	3.04µm	-5.10	182.35µm
Caffeic acid	-4.29	721.33µm	-5.08	188.39µm
Ferulic acid	-5.06	196.24µm	-5.28	134.22µm
β - sitosterol	-8.72	407.16µm	-10.87	10.75µm
Stigmasterol	-9.82	63.65nm	-11.21	6.05µm
Lupeol	-8.46	632.43nm	-11.93	1.80nm
β-Amyrin	-7.02	7.14µm	-10.36	25.54µm
Squalene	+59.65	6.05µm	-7.54	2.96µm

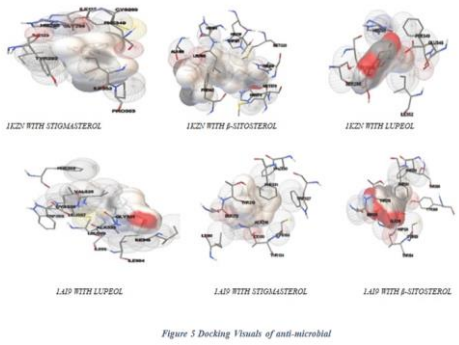


Figure 5 Docking Visuals of anti-microbial

From the above docking scores of 15 different phytoconstituents with two different mechanism possessing target its gives that this phytoconstituents have a potential Anti-microbial activity.based on the general rule of phytoconstituents has a good result based on the binding energy. They are Stigmasterol, β-sitosterol and Lupeol with their binding energy is -9.82 kcal/mol, -8.72 kcal/mol and -8.46 kcal/mol with 1KZN. They are also Lupeol, Stigmasterol and β-sitosterol with their binding energy is -11.93 kcal/mol, -11.21 kcal/mol and -10.87 kcal/mol with their 1AI9 targets respectively.And their inhibition constant also gives a good result against the respective targets.

Table 7: Docking Scores Of Hepatoprotective Activity

PHYTOCHEMICALS	Protein:3LC4		Protein:5CGJ	
	BE (kcal/mol)	IC	BE (kcal/mol)	IC
Quercetin	-6.51	16.96µm	-7.18	5.50µm
Luteolin	-8.21	966.65µm	-7.50	3.18µm

kaempferol	-8.09	1.17µm	-7.65	2.48µm
Apigenin	-8.57	523.26µm	-7.62	2.58µm
Naringenin	-8.38	714.57µm	-7.60	2.69µm
Rutin	-4.83	286.52µm	-7.79	1.94µm
Catechin	-5.19	156.26µm	-7.66	1.94µm
Gallic acid	-4.05	1.07µm	-5.82	54.64µm
Caffeic acid	-5.82	54.64µm	-4.81	299.29µm
Ferulic acid	-5.88	48.61µm	-4.93	244.43µm
β - sitosterol	-8.43	662.52µm	-9.04	234.95nm
Stigmasterol	-8.32	795.45nm	-12.69	501.66pm
Lupeol	-8.46	633.86nm	-13.29	180.20pm
β-Amyrin	-8.69	428.66nm	-13.39	61.83pm
Squalene	-5.59	79.40µm	-9.03	241.77nm

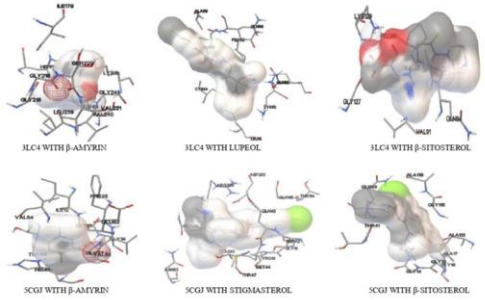


Figure 6 Docking visuals of hepatoprotective activity

From the above docking scores 15 phytoconstituents with two different proteins and that gives the plant phytoconstituents have a good Anti-diabetic activity, based on the general rule the phytoconstituents have good Hepatoprotective activity. They are β- Amyrin, Lupeol and β-sitosterol with their binding energy is -8.69 kcal/mol, -8.46 kcal/mol and -8.43 kcal/mol with 3LC4. They are also β- Amyrin, Stigmasterol andβ-sitosterolwith their binding energy is -13.39 kcal/mol, -13.29 kcal/mol and -12.69 kcal/mol with 5CGJ targets respectively.And their inhibition constant also gives a good result against the respective targets.

Admet Analysis of Abutilon Indicum

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.,

Table 8: Swiss ADME Analysis of Abutilon indicum plant phytoconstituents

PHYTO-CONSTITUENTS	MW g/mol	HBA	HBD	BIO AVAILABITY SCORE	GI ABSORPTION	BBB	LIPINSKI RULE
Quercetin	302.24	7	5	0.55	High	No	Yes
Luteolin	286.24	6	4	0.55	High	No	Yes
kaempferol	286.24	6	4	0.55	High	No	Yes
Apigenin	270.24	5	3	0.55	High	No	Yes
Naringenin	272.25	5	3	0.55	High	No	Yes
Rutin	610.52	16	10	0.15	Low	No	No
Catechin	290.27	6	5	0.55	High	No	Yes
Gallic acid	170.12	5	4	0.56	High	No	Yes
Caffeic acid	180.16	4	3	0.56	High	No	Yes
Ferulic acid	198.13	4	2	0.55	High	Yes	Yes
β - sitosterol	414.71	1	1	0.55	Low	No	Yes
Stigmasterol	412.69	1	1	0.55	Low	No	Yes

Lupeol	426.72	1	1	0.55	Low	No	Yes
β-Amyrin	426.72	1	1	0.55	High	No	Yes
Squalene	410.72	0	0	0.55	High	No	Yes

The phytoconstituents of Abutilon indicum exhibit diverse ADME profile. All the phytoconstituents have more or less equal bioavailability score ranges from 0.55 – 0.56 except rutin which bioavailability is 0.15.These making it as promising for oral administration.Phytosterol and triterpenoid like, Rutin,β-sitosterol, stigmasterol and Lupeol have the low gastro intestinalabsorbtionrate compared to other phytoconstituents. All the phytoconstituents is used for oral administration except Rutin, it requires different route of administration for bioavailability and therapeutic effectiveness.

Table 9: 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
Quercetin	0.407	No	0.499	No	No	2.471
Luteolin	0.495	No	0.499	No	No	2.455
kaempferol	0.477	No	0.531	No	No	2.455
Apigenin	0.566	No	0.238	No	No	2.45
Naringenin	0.66	No	-0.176	No	No	1.791
Rutin	-0.369	No	0.452	No	No	2.491
Catechin	0.183	No	0.438	No	No	2.428
Gallic acid	0.518	No	0.7	No	No	2.218
Caffeic acid	0.508	No	1.145	No	No	2.383
Ferulic acid	0.623	No	1.082	No	No	2.282
β - sitosterol	0.628	No	-0.621	No	No	2.552
Stigmasterol	-1.083	No	0.559	No	No	2.482
Lupeol	0.153	No	-0.502	No	No	2.563
β-Amyrin	-0.044	No	-0.558	No	No	2.729
Squalene	1.791	No	-0.553	No	No	1.893

Toxicity prediction indicates thatmost of the compounds are non-mutagenic (AMES negative) with moderate value of LD 50 values, suggesting very slightly toxicity. There is no hepatotoxic and skin sensitization phytoconstituents in Abutilon indicum which indicatesa favorable safety profile with promising oral bioavailability for several small phytosterol compounds.

CONCLUSION

The present study highlights the therapeutic potential of Abutilon indicum through molecular docking and ADMET profiling, providing a scientific basis for its multiple pharmacological activities. Docking results revealed that bioactive phytoconstituents of the plant exhibit strong binding affinities toward key molecular targets, suggesting possible roles in anti-inflammatory, antiulcer, antimicrobial, and hepatoprotective pathways. Furthermore, ADMET analysis confirmed favorable pharmacokinetic properties, including drug-likeness, absorption, and safety profiles, thereby strengthening the case for its suitability in drug development. Together, these findings not only validate the traditional medicinal use of Abutilon indicum but also open avenues for its integration into modern therapeutic strategies. Future in vivo and clinical investigations are warranted to translate these computational insights into practical applications, ensuring the plant's compounds can be harnessed effectively for human health.

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Cite this article:
Molecular Docking and Admet Analysis of The Abutilon Indicum Plant Constituent with Multiple Pharmacological Activities. *International Journal of Pharmaceutical Research & Analysis,* 2026; 16(2): 44-55.