Journal of Manmohan Memorial Institute of Health Sciences Vol 11 | Issue 1 | 2026

ORIGINAL ARTICLE

Exploring the Anti-Inflammatory Potential of *Choerospondias axillaris* Through Molecular Docking based *in silico* Pharmacological Investigation

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Received: April 09, 2026
Accepted: May 28, 2026
Published: June 5, 2026

https://doi.org/10.3126/jmmihs.v11i1.94649

How to Cite

Shrestha S, Shrestha A, Thapa RB, Adhikari P, Khanal D P, Raut *et al.* Exploring the Anti-Inflammatory Potential of Choerospondias axillaris Through Molecular Docking based in silico Pharmacological Investigation. J. Manmohan Memorial Inst. Health Sci.2026;11(1):64–69. https://doi.org/10.3126/jmmihs.v11i1.94649

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ABSTRACT

Introduction: Inflammation is an adaptive response that occurs due to harmful stimuli. Short-term inflammation is a vital protective response, but prolonged inflammation leads to various illnesses, and conventional anti-inflammatory drugs often cause adverse effects. *Choerospondias axillaris*, a medicinal plant traditionally used has demonstrated potential anti-inflammatory activity. This study aimed to evaluate the anti-inflammatory potential of different active chemical constituents through in silico investigation.

Method: In-silico method was utilized to identify potential active chemical constituents of *Choerospondias axillaris* as anti-inflammatory agents. PyRx integrated version of AutoDock, open babble, vina wizard and Biovia discovery studio were utilized to predict the scoring functions with specific protein Cyclooxygenase - II (PDB-ID: 6COX). Discovery studio visualizer and marvin sketch was used to create 2D and 3D structure, interaction, and various web server was utilized to predict and collect the data.

Result: Twenty-one active chemical constituents of *Choerospondias axillaris* were designed and docked with protein Cyclooxygenase - II (PDB-ID: 6COX. Binding affinity of the standard drug diclofenac shows -7.4 kcal/mol, two hydrogen bonds, Asn A:375 and His A: 226 with Protein [6COX], whereas AS-11 shows highest binding affinity -10.5 kcal/mol, four hydrogen bonds, Glu B: 465, Asp B: 125, Ala B:151, Tyr B:130, AS-20 shows binding affinity -10.3 kcal/mol, nine hydrogen bonds, Pro A:154, Gln A:461, Asn A:39, Glu A:465, Ala A:151, Gly A:45, Cys A:41, Tyr A:130, Leu A:152 and AS-13 shows binding affinity -10.1 kcal/mol, four hydrogen bonds, Cys B :36, Tyr B: 130, Arg B: 44, Glu B :465 with protein [6COX]. All active chemical constituents have good Physiochemical, Pharmacokinetic parameters, Lipinski's Rule (except AS-19) but almost all ligands show Nephrotoxicity and respiratory toxicity further lead optimization is needed.

Conclusion: Our in-silico investigation reveals that different types of active chemical constituents present in *Choerospondias axillaris* have different level interaction with Cyclooxygenase - II (PDB-ID: 6COX) on the basis of scoring function. Out of twenty-one ligands (AS-11) Quercetin-3-Arabinoside, (AS-13) Quercetin-3-Rhamnoside, and (AS)-20 Epicatechin Gallate might shows excellent anti-inflammatory activity on the basis of Insilco data.

Key words: **Inflammation; Anti-Inflammatory; *Choerospondias axillaris*; Molecular Docking; Cyclooxygenase – II**

INTRODUCTION

Inflammation is an adaptive response that occurs due to harmful stimuli or situations[1]. Acute and chronic inflammation serves as the body's rapid defense system, triggering an immediate protective response when tissues face injury or threat, whether from infections like bacterial, fungal or viral, physical trauma like cuts, wounds, burns, irritants or dead tissue[2]. This process activates even before the full immune response develops, working to neutralize harmful agents and limit tissue damage. Short-term inflammation is a vital protective response, prolonged inflammation is linked to various illnesses, such as rheumatoid arthritis, asthma, heart disease, neurodegenerative disorders etc[3]. Drugs like NSAIDs and Glucocorticoids are used for the management of inflammation[4]. However, the use of NSAIDs and Glucocorticoids is often limited due to their potential side effects. Hence, the search for safer, plant-derived anti-inflammatory agents has gained momentum[4].

Lapsi (*Choerospondias axillaris*), a deciduous tree from the Anacardiaceae family, is highly valued for its edible fruits[5]. Native to Nepal's hilly areas altitude: 850–1900m above sea level, this species also thrives in other Asian countries such as India, China, Thailand, Japan, and Vietnam[6]. The fruits of C. axillaris hold significant value in traditional medicine used to treat tongue infections, chest discomfort, fever, poor appetite, and heart-related issues[7]. Furthermore, scientific studies have found many pharmacological actions of *Choerospondias axillaris* including anti-inflammatory action, anti-oxidant property, immunological action, cardiovascular action, potential anti-tumor action, anti- hyperlipidemic activity, hypoglycemic action, xanthine oxidase inhibitory action etc[8].

The fruit measures approximately 3 cm in length, featuring a tart, whitish pulp and green to yellow skin[9]. It has five indentations at the top and contains a large central stone with up to five holes shown in figure - 1[9]. Lapsi fruit is rich in beneficial bioactive compounds, particularly polyphenols and flavonoids, which are known for their significant health-promoting properties[10]. Key chemical components identified so far are: gallic acid, protocatechuic acid, catechin, epicatechin, quercetin-3-O-rhamnoside, epicatechin gallate, ellagic acid, quercetin-3-O-glucoside, quercetin-3-

O-arabinoside, dihydroquercetin, quercetin, protocatechuic acid, gallic acid, 3,3'-di-o-methylellagic acid, beta-sitosterol, daucosterol, stearic acid, triacontanoic acid, octacosanol, kaempferol, salicylic acid, hydroquinone, vanillic acid, citric acid, arachidic acid, palmitic acid, ascorbic acid, cinnamic acid, sinapic acid etc[6].

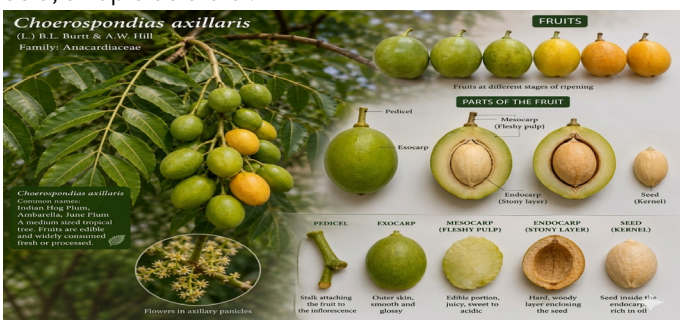


Figure 1: Different parts of the Choerospondias axillaris fruits

Molecular docking is a computational technique used to predict the optimal binding orientation, estimate the binding affinity, scoring function[11]. Molecular docking plays a key role in structure-based drug design hence It predicts the drug target interaction. This approach enables the identification and optimization of promising compounds, making drug discovery more efficient[12]. In natural product research, it helps validate traditional medicinal uses and discover new therapeutic applications for plant-derived compounds.

Therefore, the present study aims to conduct an integrative investigation of the *Choerospondias axillaris* as anti-inflammatory potential through in-silico models. This comprehensive approach is expected to validate the traditional use of *Choerospondias axillaris* and contribute to the development of novel therapeutic agents for combating acute and chronic inflammation.

METHODS

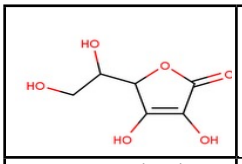
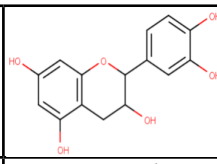
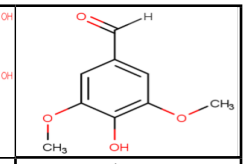
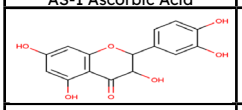
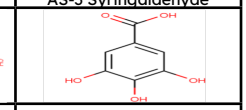
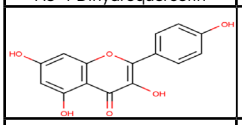
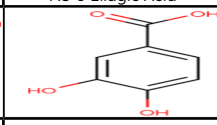
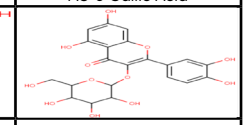
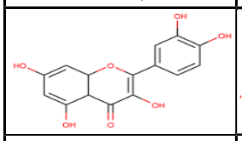
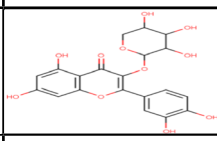
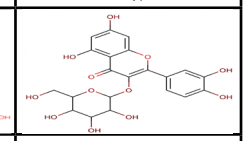
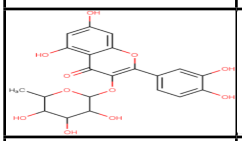
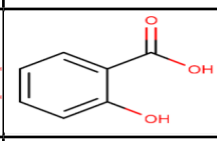
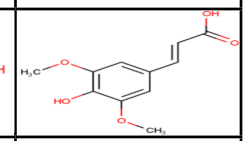
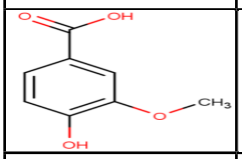
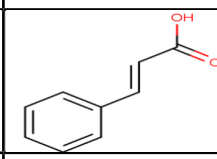
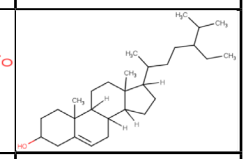
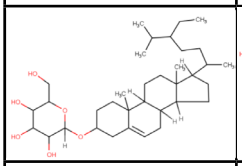
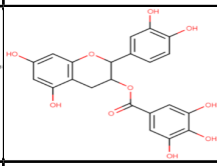
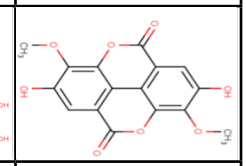
Ethics approval: The study protocol received ethical approval from the Institutional Review Committee of Manmohan Memorial Institute of Health Sciences (MMIHS-IRC), under approval number NEHCO-IRC/081/066.

Molecular Docking software: PyRx[13] and Biovia discovery studio[14] were utilized to predict the docking score and drug-receptor interaction[15]. Web-server https://www.swissadme.ch/, http://sts.bioe.uic.edu/, https://www.rcsb.org/, https://chatgpt.com/[16-17] were utilized to predict physiochemical, pharmacokinetics, biological activity and toxicological parameters.

Preparation of 3D model of Ligands: Twenty-one different ligands were selected by thorough literature review and the selected ligand structures were constructed by using Marvin Sketch in 3D SDF file format[18-19]. These files were then converted into PDB and PDBQT format using PyRx software shown in Table – 1.

Preparation and validation of target Protein: The target proteins were obtained from Protein Data Bank (http://www.rcsb.org/pdb/) on the basis of x-ray diffraction resolution, absence of mutations, and validation through the Ramachandran plot. Optimization involved cleaning the structure, removing irrelevant residues, correcting structural errors, and incorporating polar hydrogen bonds[20].Targets were selected namely Cyclooxygenase - II (PDB-ID: 6COX)[21]. The protein was validated by inbound ligand. The final refined structure was then saved in PDB format for further docking studies shown in Table - 2.

Table 1: Active chemical constituents of *Choerospondias axillaris*

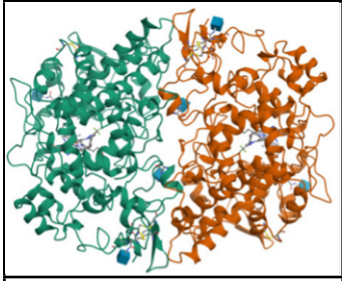
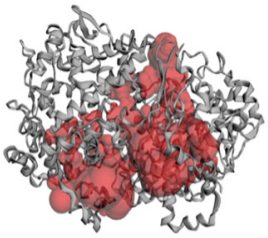
 AS-1 Ascorbic Acid	 AS-2 Catechin	 AS-3 Syringaldehyde
 AS-4 Dihydroquercetin	 AS-5 Ellagic Acid	 AS-6 Gallic Acid
 AS7- Kaempferol	 AS8- Protocatechuic Acid	 AS9- Hyperin
 AS10- Quercetin	 AS11- Quercetin-3-Arabinoside	 AS12- Quercetin-3-O-Glucoside
 AS13- Quercetin-3-Rhamnoside	 AS14- Salicylic Acid	 AS15- Sinapic Acid
 AS16- Vanillic Acid	 AS17- Cinnamic Acid	 AS18- Beta Sitosterol
 AS-19 Daucosterol	 AS-20 Epicatechin Gallate	 AS-21 3,3-Di-O-Methyl Ellagic Acid

Identification of binding pockets: Binding Pocket was identified by using Computed Atlas of Surface Topography of proteins (CASTp) (http://cast.engr.uic.edu), webserver[22]. Hence, Active binding pockets of Cyclooxygenase - II (PDB-ID: 6COX) have 175 active amino acid in chain-A 173 active amino acid in chain-B out of 587 amino acids Shown in Table - 2.

Pharmacokinetic and Toxicity Prediction: The pharmacokinetic properties of all ligands, were predicted using the SWISS ADME web server (http://www.swissadme.ch/)[23]. Furthermore, their toxicity profiles were assessed using the ProTox-II web server (https://toxnew.charite.de/)[24-25].

Biological Activity Prediction: To validate the docking results, the PASS web server (https://www.way2drug.com/passonline/) was utilized to predict the biological activity of the bioactive compounds, with a focus on antibacterial potential having the probability of activity (Pa) exceeded the probability of inactivity (Pi)[26].

Table 2: 3D Crystal structure of the Cyclooxygenase - II (PDB-ID: 6COX)[21]

PDB ID: [6COX]	Active Binding Pockets of 6COX
	
Classification: Oxidoreductase Organism: Mus musculus Expression system: Spodoptera frugiperda Mutation: No Method: X-ray diffraction Resolution: 2.80Å	175 active amino acid in chain-A and 173 active amino acid in chain-B out of 587 amino acids.

Docking methodology: Molecular docking was performed using integrated PyRx software[27]The protein structure was imported into AutoDock 4.2, converted to PDBQT format. Ligands were uploaded, their geometries were energy-minimized to obtain the most stable conformers, and then converted into PDBQT format. The docking grid parameters were set and obtained conformations were further analysed using Discovery Studio 2026[28] The binding affinity was estimated using the equation:

$$\Delta G_{Binding} = \Delta G_{Gauss} + \Delta G_{Repulsion} + \Delta G_{H\text{-}Bond} + \Delta G_{Hydrophobic} + \Delta G_{Tors}$$

Where;

ΔG_{Gauss}: Represents the dispersion of two Gaussian functions.

$\Delta G_{Repulsion}$: Accounts for repulsion beyond a threshold distance

$\Delta G_{H\text{-}Bond}$: Models hydrogen bond interactions.

$\Delta G_{Hydrophobic}$:Ramp function for hydrophobic interactions.

ΔG_{Tors}: Proportional to the number of rotatable bonds[28].

RESULTS AND DISCUSSION

Molecular docking analysis

Twenty-one active chemical constituents of Choerospondias axillaris (fruits)were designed and docked with Cyclooxygenase - II (PDB-ID: 6COX)[21] are listed in Table-3 and Figure-2. The ligand with the lowest binding energy, higher number of hydrogen bonds, shorter bond distance, and greater amino acid interactions was identified as the most promising candidate for further investigation.

Binding affinity of the standard drug diclofenac shows -7.4 kcal/mol, two hydrogen bonds, Asn A:375 and His A: 226 with Protein [6COX], whereas AS-11 shows highest binding affinity -10.5 kcal/mol, four hydrogen bonds, Glu B: 465, Asp B: 125, Ala B:151, Tyr B:130 with [6COX], AS-20 shows binding affinity -10.3 kcal/mol, nine hydrogen bonds, Pro A:154, Gln A:461, Asn A:39, Glu A:465, Ala A:151, Gly A:45, Cys A:41, Tyr A:130, Leu A:152 with protein [6COX] and AS-13 shows binding affinity -10.1 kcal/mol, four hydrogen bonds, Cys B :36, Tyr B: 130, Arg B: 44, Glu B :465 with protein [6COX] shown in Table – 3 and Figure – 2. 13 out of 21 ligands show higher scoring function as compared to standard diclofenac among these AS-11 Quercetin-3-Arabinoside, AS-13 Quercetin-3-Rhamnoside, AS-20 Epicatechin Gallate shows excellent scoring function as compare to the Salamun *et al.*[21]

Table 3: Molecular docking result of active chemical constituents of Choerospondias axillaris and standard Diclofenac with Cyclooxygenase - II [PDB-ID: 6COX]

Sn	Code Name	Bindin Energy (kcal/mol)	Number of Amino Acid
0	**DIC**	**-7.4**	Asn A:375, His A: 226
1	AS-1	-6.3	Tyr B :385 Ala B :199, His B :388
2	AS-2	-9.3	Glu B:465, Arg B:469
3	AS-3	-5.8	Cys B:47, Gly B:45, Asn B:39
4	AS-4	-9.4	Pro A:154, Cys A:47, Gly A:45, Glu A:465
5	AS-5	-9.6	Asn B:39, Glu B:465, Gln B:461, Tyr B:130, Gly B:135
6	AS-6	-6.5	Val A:523, Tyr A:385
7	AS-7	-9.1	Gly B:135, Cys B:47
8	AS-8	-6.4	Gln B:330, Gly B:235, Glu B:236, Thr B:237
9	AS-9	-9.4	Tyr B:130, Glu B:465, Gln B:42
10	AS-10	-9.5	Gly A:45, Cys A:47, Tyr A:130, Asn A:39
11	**AS-11**	**-10.5**	Glu B: 465, Asp B: 125, Ala B:151, Tyr B:130
12	AS-12	-8.9	Asp B:157, Cys B:47, Gly A :324
13	**AS-13**	**-10.1**	Cys B :36, Tyr B: 130, Arg B: 44, Glu B :465
14	AS-14	-6.2	Tyr A :385, Trp A: 387, Ala A: 202
15	AS-15	-6.7	Gln A: 369, Gln B: 370, Gln B: 372, Lys B :352, Ile B: 124, Ser B :126
16	AS-16	-6.3	Asn B:144, Lys A:333, Gly A:235
17	AS-17	-6	Tyr A:385
18	AS-18	-8.1	Arg B:61
19	AS-19	-9.5	Cys B:47, Asn B:34, Cys B:36, Pro B:154
20	**AS-20**	**-10.3**	ASN A:39, CYS A:41, GLY A:45, PRO A:154, TYR A:130, ALA A:151, GLA A:461, GLU A:465
21	AS-21	-9.5	Gln B:461, Asn B:39, Tyr B:130, Cys B:47

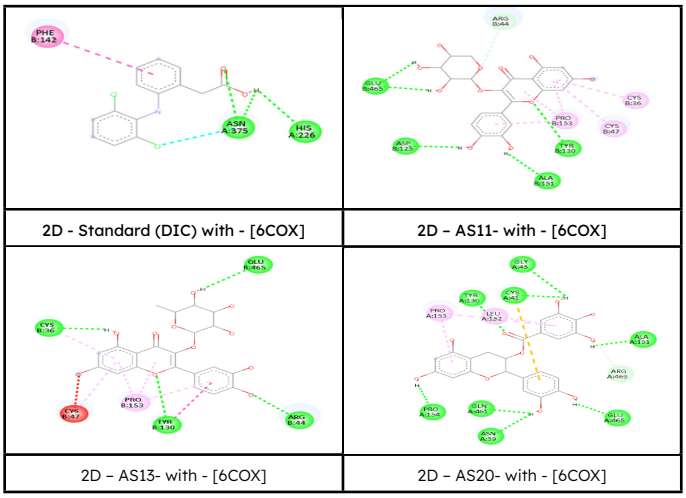


Figure 2: 2D interaction of DIC, AS-11, AS-13 and AS-20 with [6COX]

Physiochemical, Lipinski's Rule and Pharmacokinetic parameters analyses: The molecular docking, parameters were further validated by the physicochemical properties

and pharmacokinetic parameters, as presented in the Table-4. All derivatives comply with Lipinski's rule except **AS-19**, exhibiting an optimal molecular weight, hydrogen bond acceptors, and hydrogen bond donors[29]. Additionally, they demonstrate favourable lipophilic properties ranges from (-0.3 – 5.1), high GI-absorption except AS-9,11,12,13,18,19,20. Most of the ACC don't cross blood brain barrier except AS-3,14 and 17. 7 out of 21 ACC shows interaction with CYP enzyme and Lead likeness was shown by AS-2,4,5,7,10 and 21. Hence physiochemical, Lipinski's Rule and Pharmacokinetic parameters analyses shows that all ACC have good pharmacokinetic parameters.

Table 4: Physiochemical, Lipinski's Rule and Pharmacokinetic parameters

SN	Mol. Wt	RB	HA	HD	Log-p	Lip Rule	GI-Abs	BBB	CYP Inhibi-tors	Lead Like
DIC	296	4	2	2	4.5	Yes	High	No	2C9	No
AS-1	176	2	6	4	-0.3	Yes	High	No	No	No
AS-2	290	1	6	5	1.3	Yes	High	No	No	Yes
AS-3	182	3	4	1	1.6	Yes	High	Yes	No	No
AS-4	304	1	7	5	0.7	Yes	High	No	No	Yes
AS-5	302	0	8	4	0.7	Yes	High	No	1A2	Yes
AS-6	170	1	5	4	0.2	Yes	High	No	3A4	No
AS-7	286	1	6	4	1.7	Yes	High	No	2D6 1A2 3A4	Yes
AS-8	154	1	4	3	0.6	Yes	High	No	3A4	No
AS-9	464	4	12	8	1.4	No	Low	No	No	No
AS-10	302	1	7	5	1.0	Yes	High	No	2A2 2D6 3A4	Yes
AS-11	434	3	11	7	1.5	No	Low	No	No	No
AS-12	463	4	12	8	1.4	No	Low	No	No	No
AS-13	448	3	11	7	1.2	No	Low	No	No	No
AS-14	138	1	3	2	1.1	Yes	High	Yes	No	No
AS-15	224	4	5	2	1.0	Yes	High	No	No	No
AS-16	168	2	4	2	1.4	Yes	High	No	No	No
AS-17	148	2	2	1	1.5	Yes	High	Yes	No	No
AS-18	414	6	1	1	5.0	Yes	Low	No	No	No
AS-19	576	9	6	4	5.1	Yes	Low	No	No	No
AS-20	442	4	10	7	1.7	Yes	Low	No	No	No
AS-21	330	2	8	2	1.9	Yes	High	No	1A2	Yes

Biological activity prediction: The docking parameters and pharmacokinetic parameters was further validated by biological activity predicter shown in Table - 5. All of the bioactive chemical compounds had greater probability to be active (Pa) values than probability to be inactive (Pi) values except AS-1 and AS-9 have minimal Pa value. Hence AS-11 Quercetin-3-Arabinoside, AS-13 Quercetin-3-Rhamnoside, AS-20 Epicatechin Gallate shows optimal biological activity compare with the standard molecule's diclofenac.

Toxicity Prediction: Toxicological parameters, including hepatotoxicity, neurotoxicity, nephrotoxicity, Respiratory toxicity, cardiotoxicity, and cytotoxicity, were predicted listed in Table - 6. Almost all ligands lie in 4,5,6 classes. Most of the ligand shows Nephrotoxicity and respiratory toxicity. As-11,13 and 20 ligands lie in class 4 and 5, with LD50 = 5000mg/kg, and LD50 = 1000mg/kg, exhibited nephrotoxicity, respiratory toxicity, and cardiotoxicity indicating further lead optimization.

Table 5: Probability of Anti-inflammatory Activity of active chemical constituents

S.N.	Pa-value	Pi-value	Biological Activity
DIC	0,779	0,008	Anti-inflammatory Activity
AS-1	0,261	0,007	Anti-inflammatory Activity
AS-2	0,415	0,019	Anti-inflammatory Activity
AS-3	0,575	0,004	Anti-inflammatory Activity
AS-4	0,749	0,010	Anti-inflammatory Activity
AS-5	0,548	0,044	Anti-inflammatory Activity
AS-6	0,676	0,019	Anti-inflammatory Activity
AS-7	0,538	0,046	Anti-inflammatory Activity
AS-8	0,739	0,011	Anti-inflammatory Activity
AS-9	0,262	0,200	Anti-inflammatory Activity
AS-10	0,783	0,008	Anti-inflammatory Activity
AS-11	0,739	0,011	Anti-inflammatory Activity
AS-12	0,754	0,010	Anti-inflammatory Activity
AS-13	0,713	0,014	Anti-inflammatory Activity
AS-14	0,612	0,029	Anti-inflammatory Activity
AS-15	0,505	0,055	Anti-inflammatory Activity
AS-16	0,656	0,022	Anti-inflammatory Activity
AS-17	0,467	0,067	Anti-inflammatory Activity
AS-18	0,621	0,028	Anti-inflammatory Activity
AS-19	0,611	0,029	Anti-inflammatory Activity
AS-20	0,749	0,010	Anti-inflammatory Activity
As-21	0,779	0,008	Anti-inflammatory Activity

This study presents several limitations that warrant consideration in future research. Firstly, Inflammation involves multiple signalling pathways, targeting few receptors or enzyme via docking might not reflect the multifaceted nature of inflammatory diseases and only limited active chemical constituents were selected for in-silico investigation. Molecular docking and ADMET analyses revealed promising candidate compounds, lacks experimental validation such as in vitro or in vivo studies limits. Molecular docking results are predictive and may not fully represent biological interactions in complex living systems; thus, docking alone cannot confirm efficacy.

CONCLUSION

Our in-silico investigation reveals that different types of active chemical constituents present in Choerospondias axillaris have different level interaction with Cyclooxygenase - II (PDB-ID: 6COX) on the basis of scoring function. Among twenty-one ligands AS-11 Quercetin-3-Arabinoside, AS-13 Quercetin-3-Rhamnoside, and AS-20 Epicatechin Gallate shows superior scoring function compared with standard diclofenac with good physiochemical, pharmacokinetic parameters and optimal anti-inflammatory activity but

Table 6: Toxicity prediction of standard and active chemical constituents

S.N.	LD50 Mg/kg	Toxicity class	Hepato-Toxicity	Neuro-Toxicity	Nephro- Toxicity	Resp-Toxicity	Cardio-Toxicity	Cyto-Toxicity
DIC	299	3	A	IA	IA	IA	IA	IA
AS-1	3367	5	IA	IA	A	IA	IA	IA
AS-2	10000	6	IA	IA	A	A	IA	IA
AS-3	2000	4	IA	IA	A	IA	IA	IA
AS-4	2000	4	IA	IA	A	A	IA	IA
AS-5	2991	4	IA	IA	A	A	IA	IA
AS-6	2000	4	IA	IA	A	A	IA	IA
AS-7	3919	5	IA	IA	A	A	IA	IA
AS-8	2000	4	IA	IA	A	IA	IA	IA
AS-9	5000	5	IA	IA	A	A	IA	IA
AS-10	159	3	IA	IA	A	A	IA	IA
AS-11	5000	5	IA	IA	A	A	IA	IA
AS-12	5000	5	IA	IA	A	A	IA	IA
AS-13	5000	5	IA	IA	A	A	A	IA
AS-14	1034	4	A	IA	A	A	IA	IA
AS-15	1772	4	IA	IA	A	IA	IA	IA
AS-16	2000	4	IA	IA	A	IA	IA	IA
AS-17	2500	5	A	IA	A	IA	IA	IA
AS-18	890	4	IA	A	IA	A	IA	IA
AS-19	8000	6	IA	IA	A	IA	A	IA
AS-20	1000	4	IA	IA	A	A	IA	IA
AS-21	423	4	IA	IA	A	A	A	IA

Note: LD50 values are given in [mg/kg]: Class I: fatal if swallowed (LD50 ≤ 5), Class II: fatal if swallowed (5 < LD50 ≤ 50), Class III: toxic if swallowed (50 < LD50 ≤ 300), Class IV: harmful if swallowed (300 < LD50 ≤ 2000), Class V: may be harmful if swallowed (2000 < LD50 ≤ 5000) and Class VI: non-toxic (LD50 > 5000).

most of the ligands shows nephrotoxicity and respiratory toxicity. Hence on the basis of above data AS-11 Quercetin-3-Arabinoside, AS-13 Quercetin-3-Rhamnoside, and AS-20 Epicatechin Gallate might shows excellent anti-inflammatory activity, further in-vitro and in-vivo test was required to validate.

Docking can be done with more ligands and more target proteins involved behind the inflammation mechanism. Further In Vivo Studies using appropriate animal models to validate the anti-inflammatory efficacy and safety profile of bioactive compounds identified from Choerospondias axillaris. Further structural modifications may be required to optimize bioavailability and minimize toxicity of the most promising candidates.

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ACKNOWLEDGEMENT

The authors sincerely thank the Department of Pharmacy at Manmohan Memorial Institute of Health Sciences, administration team and supporting hands for supporting and encouragement throughout the research process.

AUTHOR CONTRIBUTIONS

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Pharsuram Adhikari, Bechan Raut, Dharma Prasad Khanal: Conceptualization, Methodology, Data Curation, Formal Analysis Validation, Visualization, Funding acquisition, Writing – Review & Editing.

CONFLICT OF INTEREST

The authors declare no competing interests

FUNDING

None