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Original Research Article

In-Silico Molecular Docking Study for Inhibitory Potential of Terpenoids Derivatives from *Arisotolochia indica* Root against Inflammasome *PLA2: Exploring Anti-Snake Venom Efficacy*

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Abstract: ***Background*:** Nature has endowed snakes with a formidable chemical known as venom, honed over millions of years of evolution. Snakes utilise venom to immobilise their prey and to flourish in their natural habitat. Venom is acknowledged as a highly poisonous mixture of many chemicals, such as carbohydrates, nucleosides, amino acids, lipids, proteins, and peptides. They include neurotoxic, cytotoxic, cardiotoxic, myotoxic, and various enzymatic effects. In India, the root of *Aristolochia indica* (A. indica) is employed for malarial fevers; the juice derived from the leaves of the plant is claimed to operate as a specific antidote for cobra venom. ***Purpose*:** The current work scientifically validates the ethnobotanical properties of *A.indica* root bioactive against snake venom poisoning by a pharmacoinformatic strategy targeting venom inflammasomes *PLA2*. ***Method*:** The purpose of the current study was to assess the efficiency of bioactive found in *A. indica* root for their inhibitory potential against phospholipase 2 (*PLA2*) enzyme to elicit the anti-venom potency. The Auto Dock software used a grid-based docking algorithm to determine the bond. ***Result*:** *A. indica* root found to be effective anticonvulsant agent and effectively binds to be target protein *PLA2* with binding energy of -5.53,-8.57 & -6.28 kcal/mol for aristolochic acid, aristolochene & ishwarol respectively. ***Conclusion*:** The outcome of findings revealed that terpenoid derivatives showed potent inhibitory effect on *PLA2* enzyme which reflects the efficacy of *A. indica* root as potent anti-venom agent.

Keywords: *A. Indica* Root, Anti-Venom, Molecular Docking, Aristolochic Acid, Aristolochene & Ishwarol, PLA2 Enzyme.

INTRODUCTION

Snakebite envenoming constitutes a worldwide health issue and is classified as a neglected tropical illness. It affects 2.5 million individuals annually, with fatality estimates ranging from 81,000 to 138,000. Snake venoms induce several local and systemic effects in humans, some of which are life-threatening, while others result in lasting debilitation. In the absence of prompt and efficient antivenom administration, snakebite morbidity may result in lasting impairment and deformity [1]. The clinical consequences of envenomation can be categorised into three primary diseases and pathophysiological responses: neurotoxicity, haemotoxicity, and tissue damage [2].

Neurotoxic Effects	Haemotoxicity	Tissue-damaging effects
Neurotoxic effects result from toxins that disrupt synaptic transmission, such as by hydrolysing phospholipids at the presynapse, antagonising cholinergic receptors, or obstructing certain ion channels. These effects may ultimately lead to the disruption of neuromuscular transmission, culminating, among other consequences, in respiratory paralysis [3].	Haemotoxicity serves as an overarching term for various circulatory abnormalities and haemostatic consequences induced by snake venoms. Blood clotting may be influenced so that coagulation is either expedited (i.e., procoagulation) or hindered (i.e., anticoagulation). Toxins that facilitate coagulation often influence blood clotting factors by i) activating factor X, prothrombin, and other clotting factors, ii) stimulating platelet aggregation, or iii) exerting a thrombin-like (fibrinogenolytic) action [4].	The primary cause of snakebite morbidity is tissue damage, resulting in long-term impairments such as irreversible muscle loss, contractures, hypertrophic scars, chronic ulceration, renal impairment, eye injury, and other incapacitating conditions [5].

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Aristolochia Indica **(Family**: Aristolochiaceae), popularly referred to as Indian birthwort, is a climbing woody plant with antidotal and anti-poisonous effects.

Aristolochia indica

A.indica root

Due to its exceptional therapeutic properties, it is utilised in Ayurveda and traditional medical systems. Additionally, the plant is known to possess antimicrobial, antioxidant, antibacterial, anti-inflammatory, immunomodulatory, anti-cancer, and anti-diabetic properties. The ethnobotanical literature indicates that the root possesses anti-venom effects [6]. This study aims to investigate the effectiveness of *A.indica* root terpenoid derivatives against the PLA2 enzyme, with regard to its anti-venom properties.

Experimental Work

Selection of Lead Molecules

Snakebite constitutes a significant medical, social, and economic challenge in several regions globally, particularly in tropical and subtropical countries where the bulk of the world's venomous snakes reside and access to treatment is restricted. In India, many medicinal herbs are employed as antidotes for snakebites, utilised either individually or in conjunction with other substances [7].

The increasing recognition of herbal remedies in both developed and developing nations in the twenty-first century reflects a global interest in traditional, complementary, and alternative medicine. The genus *Aristolochia*, part of the family Aristolochiaceae, has over 534 recognised species, with A. indica being a well-documented species in traditional medicine for treating various diseases [8]. A. indica is utilised for the treatment of ulcers, fever, cholera, and gastrointestinal issues in children during teething. It is regarded as an antidote for snakebites and venomous insects, increases menstrual flow, and functions as an attenuant, abortifacient, anti-inflammatory, and antibacterial agent [9-11].

The literature analysis indicates that the root of A. indica is a rich source of bioactive compounds, such as Aristolochic acid-I. Aristolochic acid-D, Aristolochic acid-N-methyl ether lactam, Aristolactam β-D-glucoside, Ishwarone, Ishwarol, Ishwarane, and Aristolochene, among others [12-14]. Aristolochic acid (AA) is a principal active component, classified as a nitrophenanthrene carboxylic acid [15]. Aristolochene is a bicyclic hydrocarbon classified under the eremophilene group of sesquiterpenes [16]. Ishwarol, a new tetracyclic sesquiterpene, is identified in the root of A.indica [17]. Previous studies indicated that several extracts of A. indica roots were assessed for their anti-inflammatory, antipruritic, and mast cell stabilising activities [18]. Terpenoids are shown to possess several pharmacological activities, including antibacterial, antifungal, antiparasitic, antiviral, antiallergenic, antispasmodic, antihyperglycemic, anti-inflammatory, and immunomodulatory effects. They have also been identified as beneficial in the prevention and treatment of several disorders, including cancer. Notwithstanding the extensive ethnomedicinal and pharmacological data about the efficacy of plant extracts as antivenoms, advancements in the isolation and characterisation of bioactive chemicals remain unimpressive. Triterpenes and sterols exhibiting antivenom effects [19]. Sesquiterpenes are notable oily compounds widely distributed in plants, lately receiving attention for their many pharmacological actions, including anticancer, anti-inflammatory, antibacterial, and antiviral properties [20]. In light of the potential of terpenes for anti-inflammatory action and as an antidote for snake venom, Aristolochic acid, Aristolochene, and Ishwarol were selected as lead compounds for the current work.

Description of Selected Lead Molecules [21-26]

Description	**Aristolochic acid**	**Aristolochene**	**Ishwarol**
Molecular formula	$C_{17}H_{11}NO_7$	$C_{15}H_{24}$	$C_{15}H_{24}O$
Synonym	8-Methoxy-6-nitrophenanthro[3,4-d][1,3]dioxole-5-carboxylic acid.	(4R,4aS,6R)-4,4a-dimethyl-6-prop-1-en-2-yl-2,3,4,5,6,7-hexahydro-1H-naphthalene.	**(**5R,6S)-5,6,9 trimethyltetracyclo[7.2.1.01,6.08,10]dodecan-2-ol**.**

Description	Aristolochic acid	Aristolochene	Ishwarol
Molecular weight	341.27 g/mol	204.35	220.35 g/mol
Pharmacology	It is used for fever, worms, skin disease and snake bite. Gastric stimulant and in the treatment of cancer, lung inflammation, dysentery, snake bites, antimicrobial activity, anti-arthritis activity, anti-allergic activity and anti-oxidant property.	Phospholipase activity, Anti-inflammatory Anti-hemorrhagic Anticoagulant activity Enzyme inhibitory Potential.	Used in dry cough, joints pain, inflammation, biliousness, dysphoea of children, snake bite and also used as abortifacient.

Selection of Target Receptors

Proteins and peptides are the principal components of snake venom that largely facilitate prey immobilisation and lethality through hypotension and paralysis.

Phospholipase A2

PLA2s are an extensively researched family of venom proteins, focussing on their structural categorisation and the mechanisms by which they provoke immunological responses following envenomation. They are esterolytic enzymes that hydrolyse glycerophospholipids, leading to the production of lysophosphatidic acid and arachidonic acid. PLA2s are classified into groups I and II based on the existence of disulphide bonds. Group I and II PLA2s are typically present in Elapid and viper venoms, respectively. Reports suggest that snake venom phospholipase A2s (svPLA2) elicit several pharmacological effects, including haemorrhage, oedema, myotoxicity, neurotoxicity, cardiotoxicity, and tissue destruction [27]. Snake venom, especially phospholipase A2 (PLA2), induces significant pathogenic consequences, requiring the creation of effective treatment strategies. Consequently, the inhibitory ability of bioactive phytoconstituents derived from certain medicinal plants on PLA2 is of interest. Consequently, PLA2 was selected as the target receptor for the present investigation.

Designing of *In-Silico* Molecular Docking Protocol

Molecular docking studies are essential for comprehending antivenom efficacy by clarifying the interactions between bioactive chemicals and venom enzymes. These investigations facilitate the identification of possible inhibitors of enzymes such as *Phospholipase A2*, a critical target in snake venom, hence advancing the development of efficient antivenoms. Through the examination of binding affinities and interactions, researchers can elucidate the therapeutic potential of natural phytocomponents, which may provide protective benefits against the deleterious impacts of snake venom.

Scientific Validation of Anti-Venom Potential Targeting against PLA2 Enzyme

Molecular Docking Studies

Ligand Preparation

2D Structure of aristolochene, aristolochic acid and Ishwarol were drawn using ChemSketch [28], the two-dimensional structure of the prepared ligand was converted into their 3-D structures optimized with 3D geometry. The optimized structure was saved in PDB format for AutoDock compatibility. The basic structures of the prepared ligand were given below:

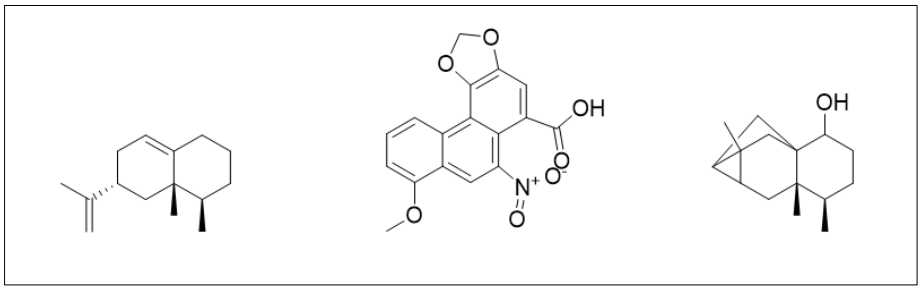


Figure 1: 2D structure of aristolochene, aristolochic acid and Ishwarol

Preparation of the Grid File

The regions of interest used by Autodock were defined by considering grid area by making a grid box around the active sites. Grid box plays a central role in process of docking as it is made to cover all the amino acids present in active sites necessary for binding other than those present in receptor. Grid box has 3 thumbwheel widgets which let us change the number of

points in the x, y and z dimensions. The spacing and grid points for all the considered receptors in the current study are given in table 1 [29, 30].

Table 1: Grid parameters used in current docking analysis of PLA2

S. No.	Receptor	x-axis	y-axis	z-axis	Spacing	x center	y center	z center
1	PLA2	50	50	50	0.386	14.627	30.229	16.421

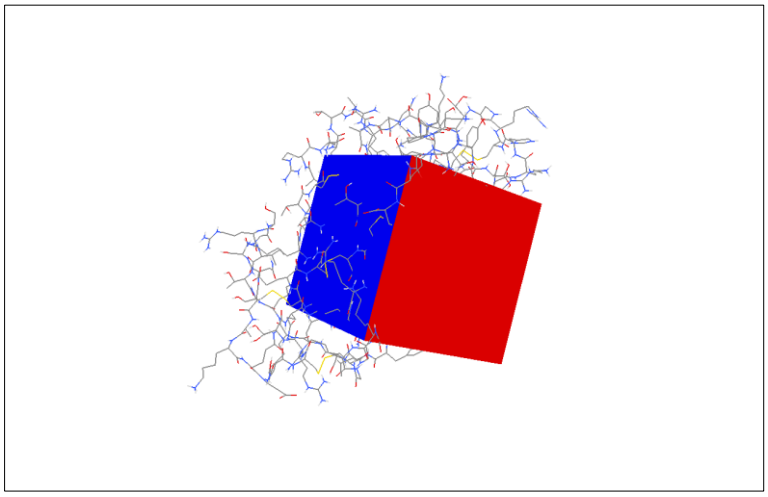


Figure 2: Grid box covering all active sites in PLA2 receptor

Preparation of the Docking File

All the calculations were carried out by using Autodock 4.2 as docking tool. The visualization and other programs necessary for docking studies were performed out by means of Pymol, Chimera, DS visualizer, MMP Plus [31-33].

Docking Study

Crystal Structure

The crystal structure of the protein consisting of PLA2 receptor is downloaded from the Protein Data Bank portal. All the primary information regarding all the receptor's structure was registered in the Protein data bank [34-36]. The complex ligand was separated by using Chimera software for all the target receptors.

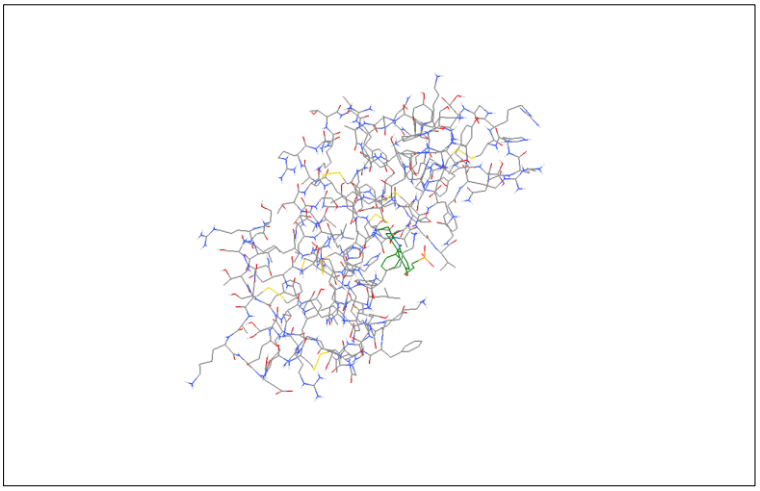


Figure 3: Crystal structure of PLA2 receptor (PDB ID-3u8d)

Processing of Protein

All the downloaded receptor proteins are having only one chains, i.e. chain A, which has been selected for experimental purpose and complex ligand was removed from it. The bound ligand was separated from the macromolecular complex by using software Chimera [37-40].

Molecular Docking Simulation Studies

Docking of ligands like aristolochene, aristolochic acid and Ishwarol against PLA2 receptor was performed by Autodock. All the bonds of each ligand were kept flexible, while no residues in receptor were made flexible [41, 42].

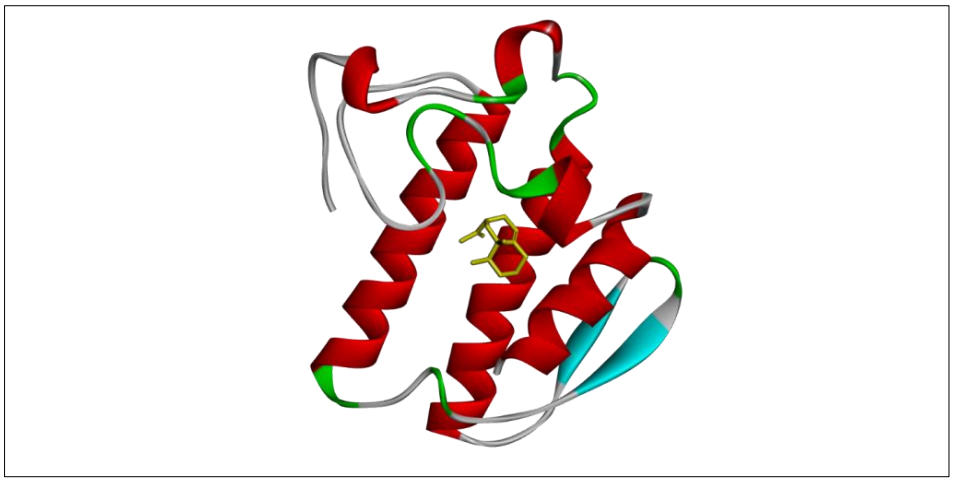


Figure 4: Binding mode of aristolochene within the active site of PLA2 receptor

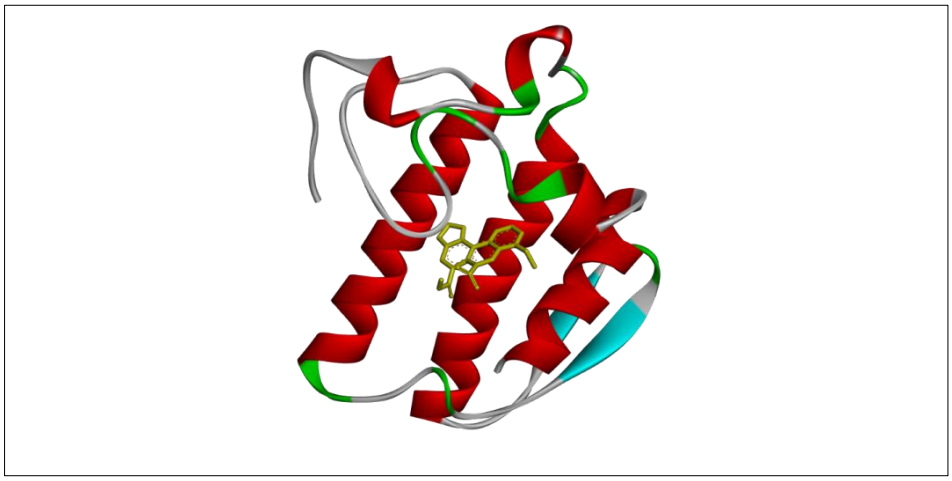


Figure 5: Binding mode of aristolochic acid within the active site of PLA2 receptor

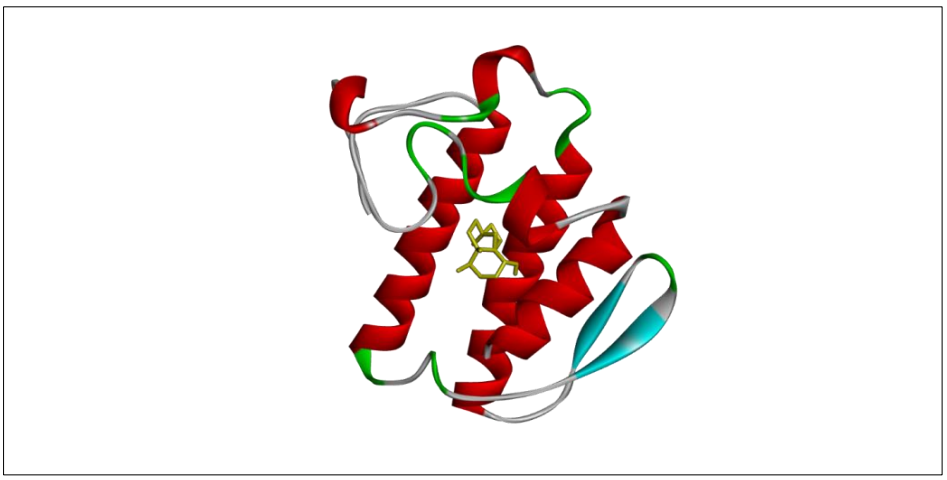


Figure 6: Binding mode of Ishwarol within the active site of PLA2 receptor

Toxicity & ADME-T Studies

The ligand molecules viz. aristolochene, aristolochic acid and Ishwarol were studied by online program OSIRIS, for prediction of presence of any toxic group as well as presence of any toxic group and ADME-T properties [43].

RESULT AND DISCUSSION

Venomous snakebites constitute a neglected tropical illness that results in hundreds of thousands of fatalities or enduring bodily and psychological disorders each year in the developing nations. Inadequate data about geographical variation in snakebite risk, occurrence, human susceptibility, and accessibility to

medical care significantly hampers efficient on-ground management. There is an immediate necessity to gather data, bridge knowledge deficiencies, and resolve practical management issues. Historically, societies have maintained the knowledge of herbal therapeutic cures transmitted over generations. Ethnomedicinal plants have historically been utilised in traditional snakebite remedies, presenting promise as supplementary therapies due to their capacity to neutralise venom poisons, especially in areas with restricted access to standard antivenoms. The venom comprises a complex amalgamation of active substances, primarily proteins and peptides, which disrupt various metabolic processes in humans or other victims of the venom. The constituents comprise phospholipase A2, L-amino acid oxidases, acetylcholinesterases, cytotoxins, mycotoxins, serine proteinases, metalloproteinases, hyaluronidases, phosphomonoesterases, phosphodiesterases, cardiotoxins, nucleosidases, hemorrhagins, neurotoxins, and coagulants.

Aristolochia indica (Family: Aristolochiaceae), popularly referred to as Indian birthwort, is a climbing woody plant with antidotal and anti-poisonous effects. Due to its exceptional therapeutic properties, it is utilised in Ayurveda and traditional medical systems. Additionally, the plant is known to possess antimicrobial, antioxidant, antibacterial, anti-inflammatory, immunomodulatory, anticancer, antidiabetic, and antivenom effects. The root is a rich source of bioactives such as Ishwarane, aristolochene, aristolindiquinone, aristololide, 2-hydroxy-1-methoxy-4H-dibenzoquinoline-4,5-(6H)-dione, cephradione, aristolactum IIa, and β-sitosterol-β-D-glucoside. Aristolactam glycoside I, stigmastenones II and III, methylaristolate, ishwarol, ishwarone, aristolochene; lignin, savinin. Terpenoids are shown to possess several pharmacological activities, including antibacterial, antifungal, antiparasitic, antiviral, antiallergenic, antispasmodic, antihyperglycemic, anti-inflammatory, and immunomodulatory effects. They have also been identified as beneficial in the prevention and treatment of several disorders, including cancer. Triterpenes and sterols exhibiting antivenom effects. This work aims to evaluate the antivenom efficacy of a chosen lead chemical against the *PLA2* inflammasome present in snake venom, considering the pharmacological potential of terpenoids. *PLA2* is among the most well examined enzymatic poisons found in snake venoms. Snake venoms are the primary source of Group I and Group II secretory phospholipase A2. The venom phospholipase A2 is a diminutive protein with a molecular mass of around 13–15 kDa. The enzyme facilitates the hydrolysis of phospholipids at the sn-2 location, yielding lysophospholipids and free fatty acids. It necessitates Ca2+ for its catalytic functions. The venom PLA2 exhibits presynaptic or postsynaptic neurotoxicity, systemic or local myotoxicity, cardiotoxicity, suppression of platelet aggregation, anticoagulant properties, and induces oedema. The neurotoxicity caused by venom is believed to result from the β-neurotoxin, a PLA2 enzyme that obstructs pre-synaptic neuromuscular transmission.

Finding of Current Investigation

The literature review demonstrates that *A.indica* root is a substantial source of terpenoids. The scientific validation of the bioactive compounds in *A. indica* root, showing effectiveness against snake venom, was investigated by *in-silico* molecular docking. Consequently, aristolochic acid, aristolochene, and ishwarol were selected as lead molecules targeting the *PLA2 enzyme*. The findings of the present study demonstrate that the chosen lead compounds are efficacious in treating snake venom, exhibiting binding affinities to the *PLA2* target protein with binding energies of -56.53, -8.57, and -6.28 kcal/mol for aristolochic acid, aristolochene, and ishwarol, respectively. The result was documented in Table 2. The binding mode of lead molecules and the target ligand is illustrated in Figures 4-6. The grid parameter for *PLA2* docking is presented in Table 1. Figures 7-12 depict the two-dimensional and three-dimensional interactions of the chosen chemical. The affinity of lead compounds for the receptor was found to be very similar. The interaction of aristolochic acid, aristolochene, and ishwarol with the active site of PLA2 is shown as follows:

Compound	**Binding against *PLA2***					
Binding mode	**Conventional Hydrogen bounding**	**π-alkyl**	**Alkyl**	**Week Vander's interaction**	**π-donor H-bond**	**π – π T shaped**
Aristolochene	-------	His47 Cys28 Phen98	Ala17 Phen5 Cys44	ILE9,Tyr21 Gly29,Gly22 Ala18,Leu2 His6	-----	------
Aristolochic acid	Val30	Ala17	His6	Cys62,Tyr51 Leu2, Ala18 Gly22,Tyr21 ILE9,Phe98, Cys28,Cys44 Asp48	His47 Gly29	Phen5
Ishwarol	---------	Phen5 Cys28 ILE9 Ala17	Leu2	His6, Phe98 Tyr21,Gly22 Glu29,Ala18	------	------

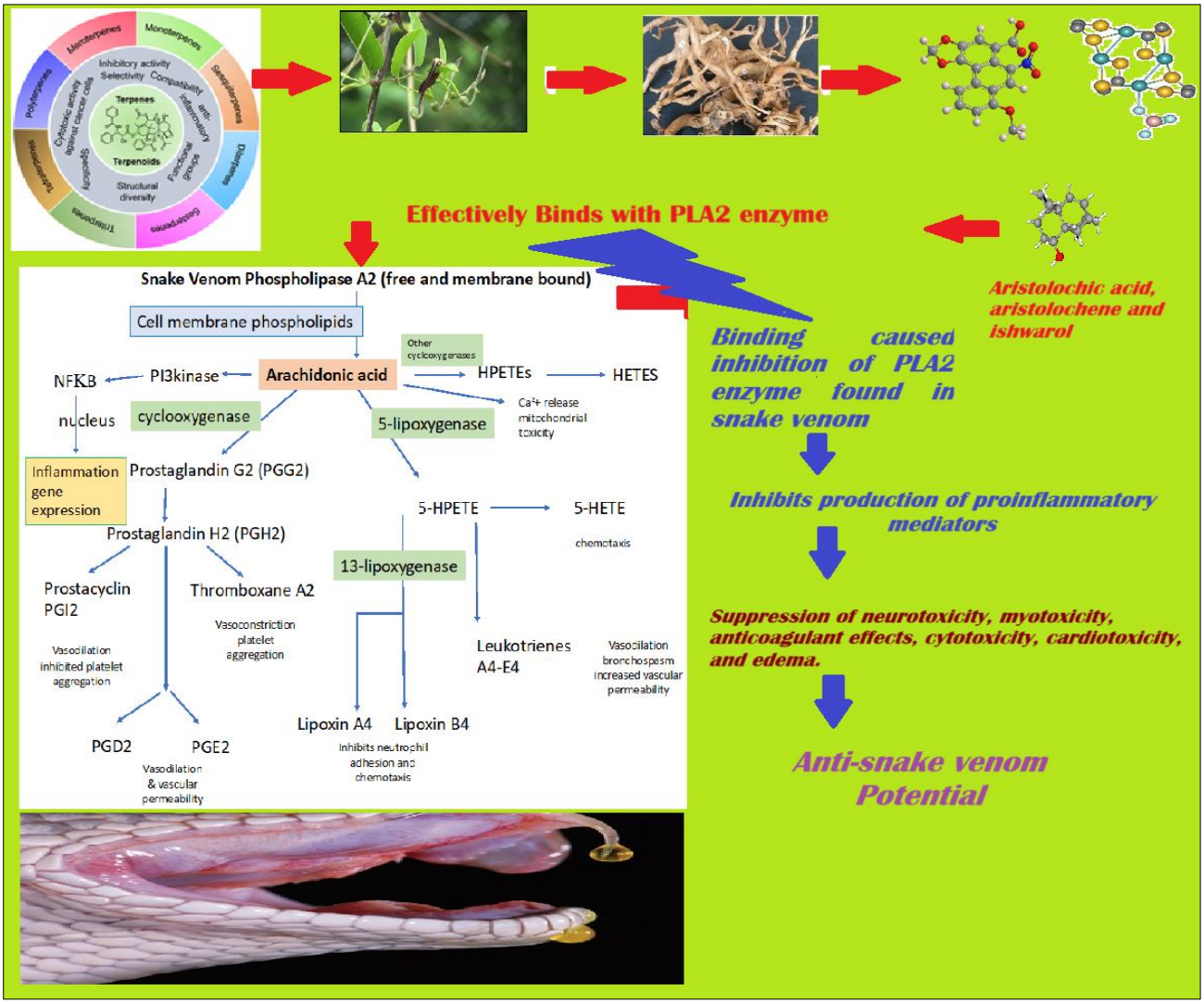
The interaction results indicated that lead molecule aristolochene and ishwarol attach at comparable positions by typical hydrogen, alkyl, π-alkyl and vander waal's interactions, whereas aristolochic acid has affinity toward receptor *via* conventional H-bonding, alkyl, π-alkyl, π-donar H bond, π- π- T shaped and vander waal's demonstrating a synergistic effect of selected molecules from *A.indica root* in exerting protective action against snake venom. The pharmacokinetic profile indicates a favourable pharmacokinetic profile; however, it also presents significant hazardous consequences, including mutagenicity, tumorigenicity, and reproductive toxicity. The pharmacokinetic and toxicity profiling data of ligands such as aristolochic acid, aristolochene and ishwarol are presented in Figures 13-15 and Tables 3-5. All ligand compounds have demonstrated promising docking scores theoretically.

CONCLUSION

The findings of the present investigation revealed that the chosen lead compounds (aristolochic acid, aristolochene, and ishwarol) exhibited substantial inhibitory efficacy against the PLA2 inflammasome, providing protective effects against snake venom. The present study demonstrates the ethnobotanical significance of A. indica root, facilitating drug development.

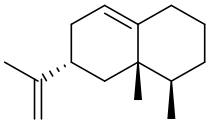
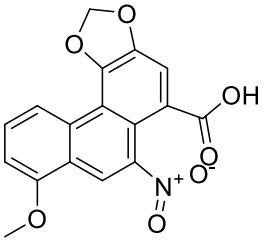
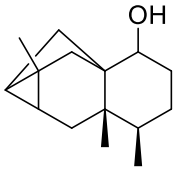
Divulgence of Investigation

The finding mechanism of action of the chosen lead molecule against PLA2 inflammasome is presented as follows:



Proposed Mechanism of Action of Terpenoid Derivatives of *A.Indica* against Snake Venom

Table 2: Results of docking of ligands like aristolochene, aristolochic acid and Ishwarol against PLA2 receptor

S. No.	Compound Name	Structure	*PLA2*
1	***Aristolochene***		-6.53
2	***Aristolochic acid***		-8.57
3	***Ishwarol***		-6.28

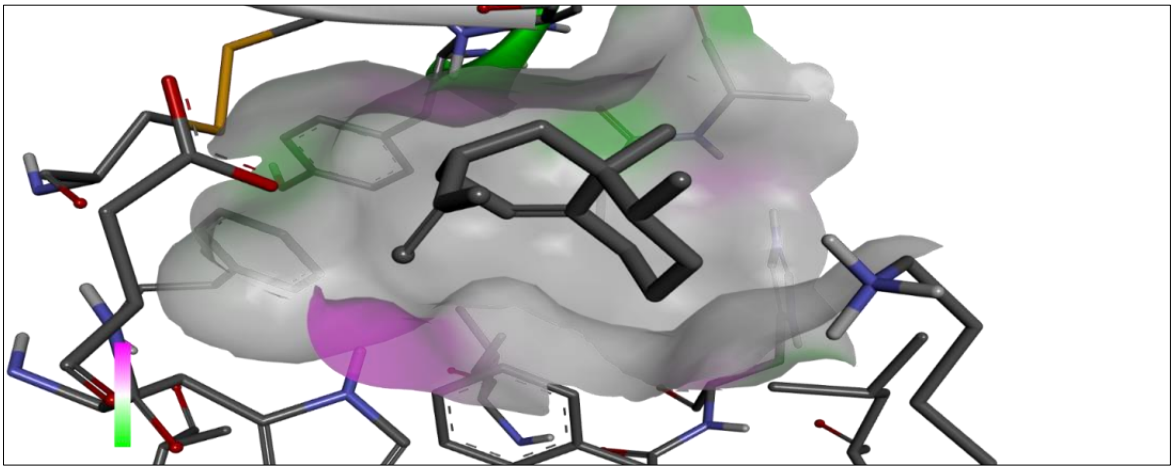


Figure 7: Three-dimensional binding mode of aristolochene within the active site of PLA2 receptor

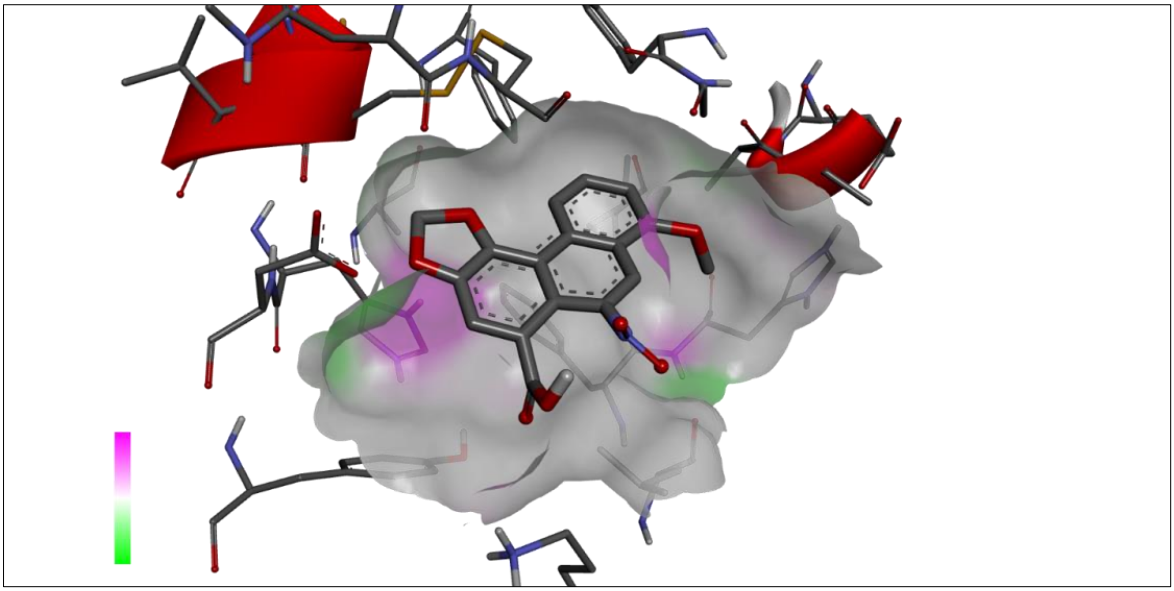


Figure 8: Three-dimensional binding mode of aristolochic acid within the active site of PLA2 receptor

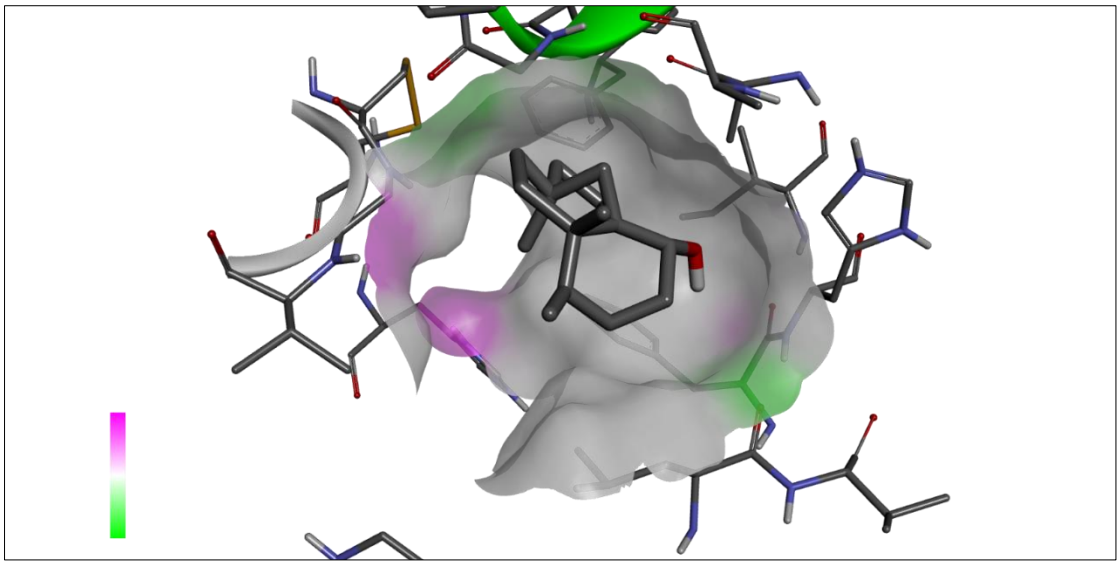


Figure 9: Three-dimensional binding mode of Ishwarol within the active site of PLA2 receptor

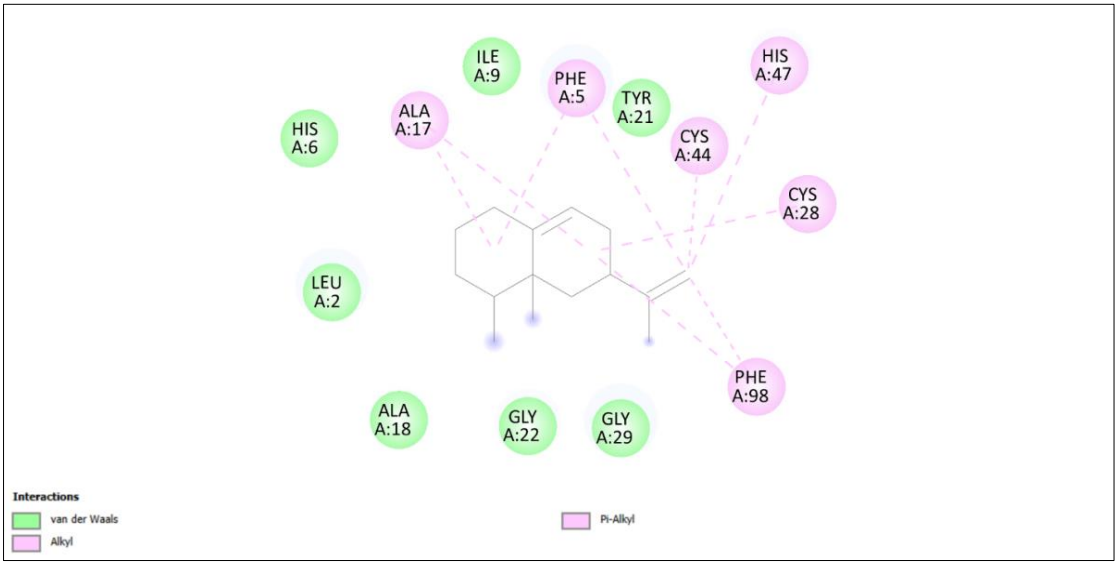


Figure 10: Two-dimensional binding mode of aristolochene within the active site of PLA2 receptor

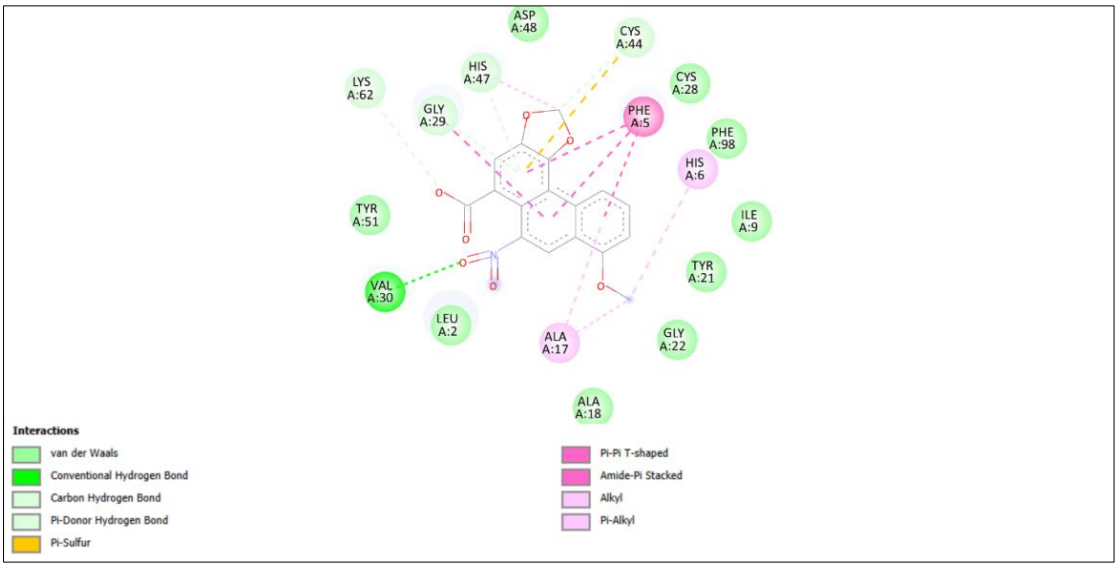


Figure 11: Two-dimensional binding mode of aristolochic acid within the active site of PLA2 receptor

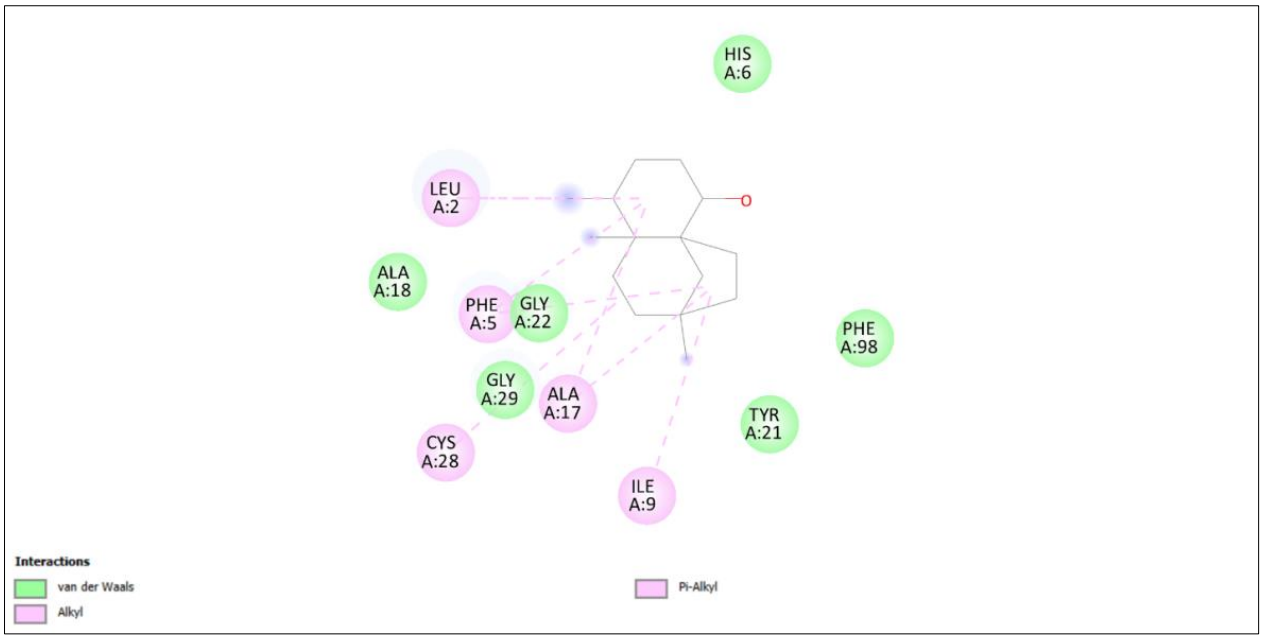


Figure 12: Two-dimensional binding mode of Ishwarol within the active site of PLA2 receptor

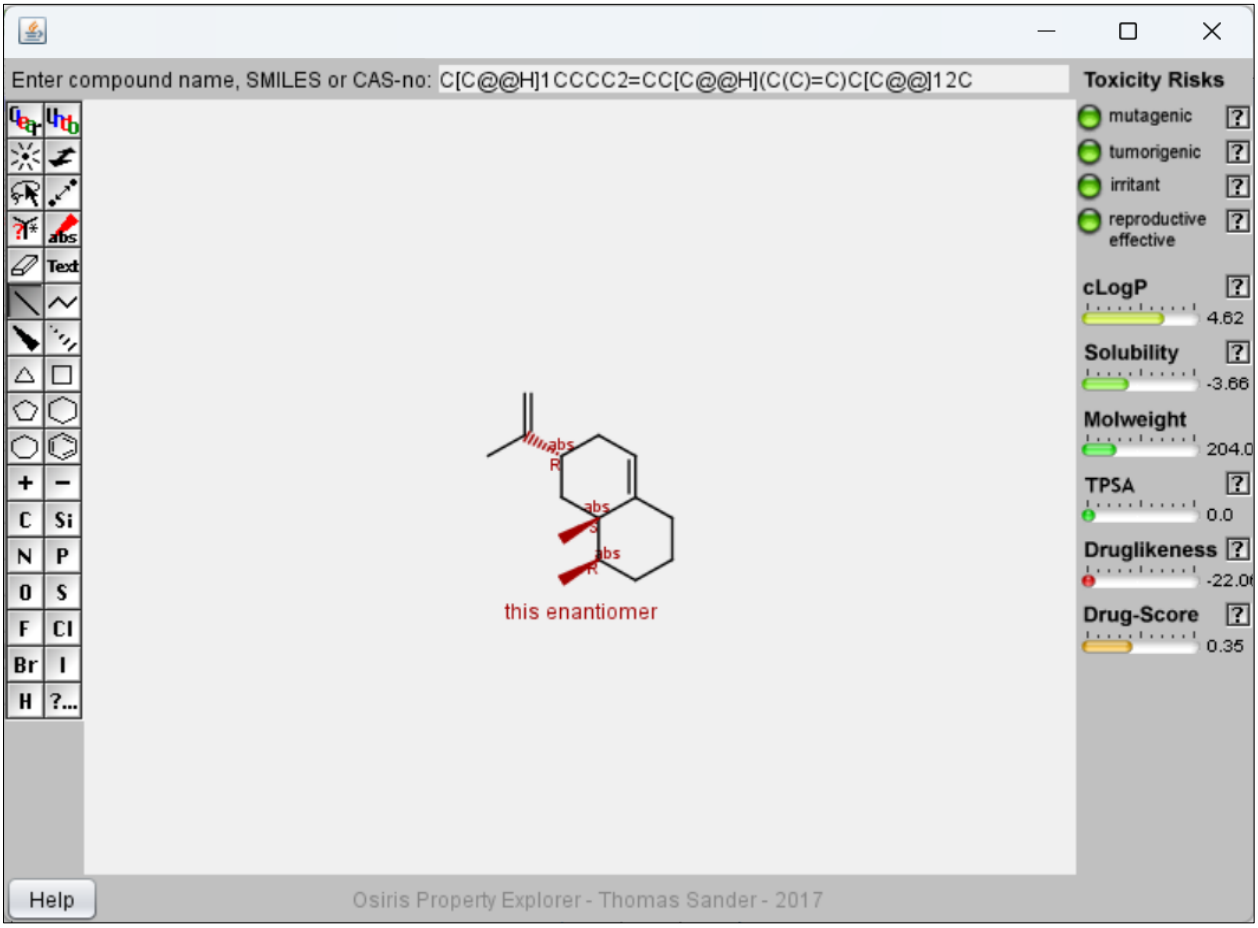


Figure 13: Pharmacokinetic and toxicity profiling of aristolochene

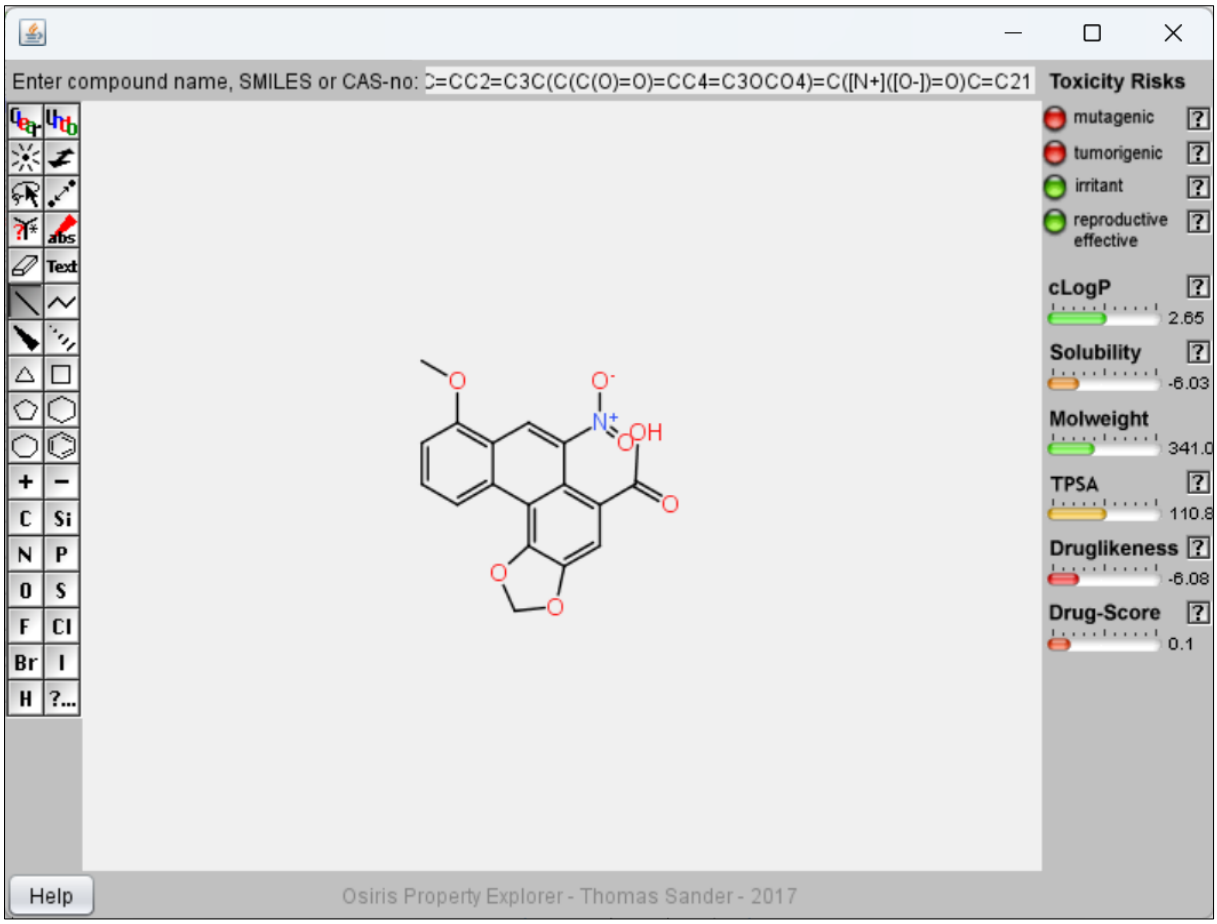


Figure 14: Pharmacokinetic and toxicity profiling of aristolochic acid

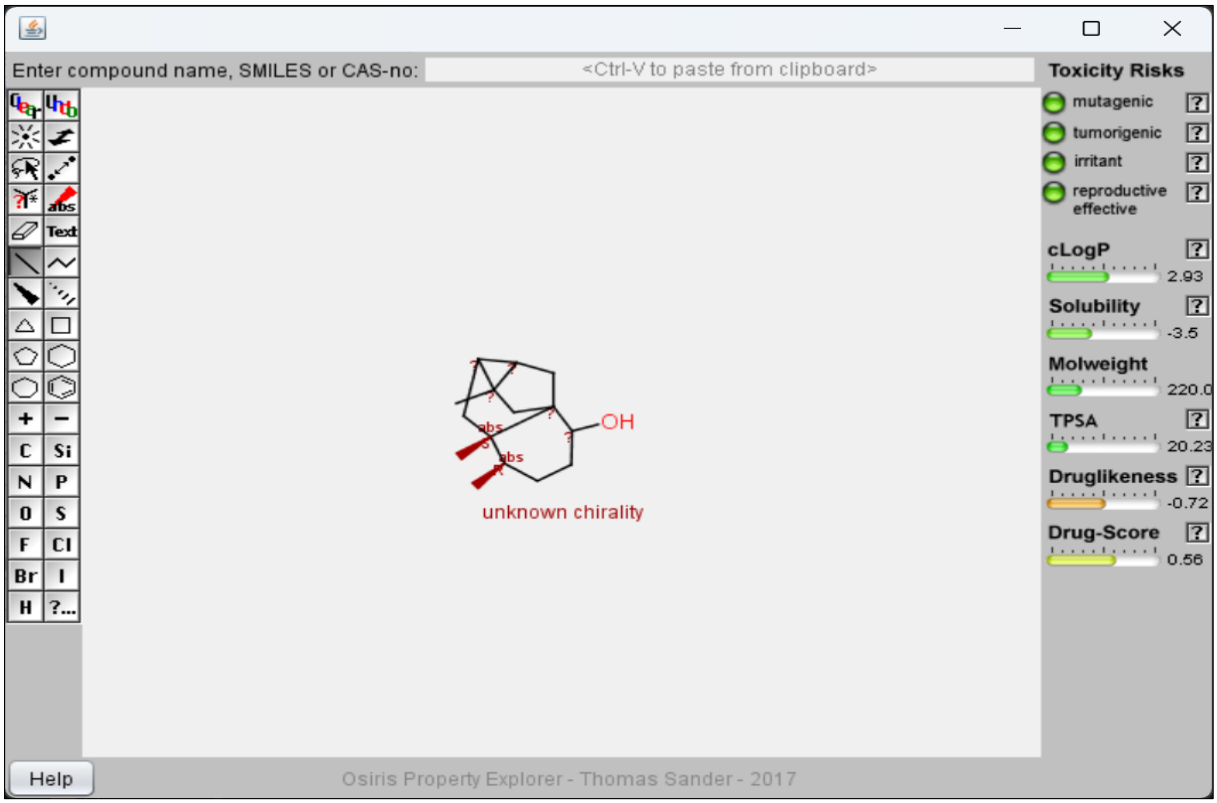


Figure 15: Pharmacokinetic and toxicity profiling of Ishwarol

Table 3: Pharmacokinetic Profiling of lead molecules

Compound	ADMET			
	Mutagenic	Tumorigenic	Irritant	Reproductive effectivity
Aristolochic acid	Mild	Mild	NO	No
Aristolochene	NO	NO	NO	No
Ishwarol	NO	NO	NO	No

Table 4: Lipinski Properties of lead molecules

Compound	*cLogP*	Solubility	Mol.wt.	TPSA	Drug likeness	Drug score
Aristolochic acid	2.65	-6.03	341	110.8	-6.08	0.1
Aristolochene	4.62	-3.66	204	0	-22.04	0.35
Ishwarol	2.93	-3.5	220	20.23	-0.72	0.56

Table 5: Drug likeness of lead molecules

Compound	Lipinski rule of five	H bond donar(<5)	H bond acceptor (<10)
Aristolochic acid	Yes	1	7
Aristolochene	Yes	0	0
Ishwarol	Yes	1	1

REFERENCE

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