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GC-MS and Molecular Docking Analyses of *Lophira lanceolata* for Hepatitis Therapeutics

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Abstract: Hepatitis which is a liver disorder is among the serious health challenges. However, current approaches used in the treatment of hepatitis and other liver disorders has some limitations and side effects. *Lophira lanceolata* Tiegh. ex. Keay (Ochnaceae) [*L. lanceolata*] is one of the plants often used in the treatment of liver disorders, though not fully proven scientifically. This study aimed to evaluate the methanol leaf extract of *L. lanceolata* for its hepatitis therapeutic potentials. The specific objective of the study was to identify and evaluate the compounds from the leaves of *L. lanceolata* with hepatoprotective potentials. Molecular docking and GC-MS analyses were used to test the potential of the compounds for direct hepatitis treatment. The leaves were cut, air dried, and pulverized. The pulverized leaves (1 kg) were cold macerated with methanol (100%) for 48hrs and filtered. The filtrate was concentrated using a rotary evaporator at 40 ^{o}C under reduced pressure, to obtain the methanol leaf extract (ME). The characterization of the bioactive constituents of *L. lanceolata* was analyzed using an Agilent HP-7890A Gas Chromatograph. The ME was subjected to Gas Chromatography-Mass Spectrometry (GC-MS). The unknown GC-MS peak value and chromatogram were compared with those from the Universität Düsseldorf Library database. Molecular docking simulation was performed using three target proteins responsibly for inflammation, oxidative stress, and hepatitis. The GC-MS analysis of the ME revealed the presence of pharmacological compounds and docking assay of the ME shows anti-inflammatory, antioxidant and anti-hepatitis compound than Silymarin. Drug-likeness evaluation demonstrated that most of the compounds conform to Lipinski's rule of five, hence they are good oral drug candidates for hepatitis. This study concludes that *L. lanceolata* used in treating liver disorders contains compounds with potential therapy against hepatitis.

Keywords: *GC-MS Analysis, Lophira lanceolata, Molecular Docking, Hepatitis*

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I. INTRODUCTION

The liver is one of the body's most essential organs. It is the site of drug metabolism and storage of nutrient reserves. It is a significant organ with many diverse functions including detoxification, excretion of hydrophobic metabolites, synthesis of plasma proteins, and storage of bile acids (Das *et al.*, 2025). Damage to this organ causes inflammation, known as hepatitis. Liver diseases are a significant global health burden, with various hepatotoxic agents like carbon tetrachloride (CCl4), paracetamol (PCM), doxorubicin (DOX), and others induce deleterious effects on hepatic function (Omale *et al.*, 2026). Hepatitis is an inflammatory condition in the liver caused by viral or non-viral factors, mainly categorized as five distinct viruses (hepatitis A, B, C, D, E), while their infection routes are different and recurrently induce a various course of disease (Oh *et al.,* 2020). According to the World Health Organization, the African continent accounts for 26% of the global burden of disease due to hepatitis B and C, with 125,000 deaths. Hepatitis is contracted by 5 to 10% of the African population (World Health Organization, 2016).

Lophira lanceolata is a tree of the tropical and subtropical regions. It is a common tree in Cameroun, Nigeria and Sudan. It often grows gregariously on fallow land at the edge of forests. It is a tree of 8 to 10 m tall, straight or twisted, with leaves alternate, clustered at the end of short straight branches, glabrous, bright and blade oblong-lanceolate. The bark surface is corky grey (Boniface *et al.*, 2020). *Lophira lanceolata* is used in traditional medicine to treat several illnesses. The decoction of the fresh leaves is administered

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orally against headaches, dysentery, diarrhoea, cough, abdominal pains and cardiovascular diseases. It is also used on skin to cure wounds (Arbonier, 2000).

The molecular docking method, widely employed in drug discovery, provides crucial insights into the interaction of small molecules with target receptors at the molecular level (Das *et al.*, 2025). This approach is precious in understanding drug mechanisms, often challenging to decipher using conventional treatments (Bhunia & Saxena, 2021). Additionally, GC-MS analysis facilitates the identification and characterization of complex organic compound mixtures in natural extracts (Muchiri & van Breemen, 2021). GC-MS elucidates the chemical composition of L. lanceolata leaf extracts by separating individual constituents according to their physicochemical characteristics and identifying them via mass spectrometry, thereby aiding in identifying potential agents (Yadav & Eswari, 2023). This study aimed to evaluate the methanol leaf extract of *L. lanceolata* for its hepatitis therapeutic potentials. The objective of the study was to identify and evaluate the compounds from the leaves of *L. lanceolata* with hepatoprotective potentials.

II. MATERIALS AND METHODS

➢ *Materials*

- *Collection and Preparation of Plant Material*

Fresh leaves of *L. lanceolata* leaves were collected from *L. lanceolata* plant. Fresh leaves of *L. lanceolata* were hand sorted to remove any dust and other contaminants and air dried at room temperature of 26ºC for 4 weeks away from direct sunlight. The dried plant materials were broken into smaller bits with a wooden mortar and pestle and pulverized into fine powder with a commercial blender 8011E model 38BL 41 and the dry leaf powder was about 1.07 kg, this was stored in airtight containers prior for extraction.

- *Extraction of Plant Material*

About 1.00 kg of the leaves of *L. lanceolata* was extracted with methanol by cold maceration for 48 h and the mixture agitated each day at intervals to ensure good and complete extraction. Thereafter, the mixture was pre-filtered using Whatman filter paper No.42 (125 mm) after which the filtrate was re-filtered through cotton wool and the marc was repeatedly washed with fresh solvent until the filtrate became clear. The filtrate was concentrated in a rotary evaporator under reduced pressure at 40ºC to obtain 121.20 g (12.12% w/w) of the methanol extract (ME). The yield of the extraction process was calculated using the relation:

$$\textbf{\% yield} = \frac{\textit{weight of the extract}\,(g)}{\textit{weight of the powdered}\,(g)} \times 100$$

➢ *Gas Chromatography-Mass Spectroscopy (GC-MS) of L. lanceolata Leaf.*

The characterization of the bioactive constituents of ***L. lanceolata*** was analyzed using an Agilent HP-7890A Gas Chromatograph (Agilent Technologies, Palo Alto, CA, USA) was carried out on an Agilent HP 7890A gas chromatograph (Technology model MSD = 5975C detector) Agilent Technologies, Injector: 7683B Series, Ionization energy: 70 eV, Palo Alto, CA, USA). Initial temperature = 100^0C held for 2 min, final temperature = 270^0C at the rate of 1 O^OC/min. A 1 ml of the various fractions of the extract was injected. Temperature of heater was set at 250^0C, pressure 3.2652 psi, mode type slit less, column type (HP 5MS: 30m x 320 gm x 0.25 gm) and carrier gas (Helium, 99.9999% purity, flow rate = 1.4963 ml/min; average velocity = 45.618 cm/s).

➢ *Identification of Compounds*

The constituent compounds were determined by comparing their retention times and mass weights with those of authentic samples obtained by GC (Adams: 2001). GC-MS interpretation on mass spectrum was conducted using the database at Institute of Pharmaceutical Biology Universität Düsseldorf. Then the phytochemicals were identified based on the hits returned after comparing the unknown peak value and chromatogram from GC-MS against the known chromatogram peak value from the Universität Düsseldorf Library database. Subsequently, the details about their molecular formula, molecular weight, structure were also obtained.

➢ *In Silico Molecular Docking Assay*

The molecular docking algorithm AutoDock Vina and Discovery Studio Visualizer (BIOVIA 2025) software were used in the docking investigation to determine the activity of the newly synthesized compounds against a protein target and to identify the potential mode of action. Based on the number of hydrogen bond interactions and the scoring mechanism, a particular position was chosen for additional examination. X, Y, and Z coordinates were used to assess the binding site properties and define the active binding site using the ligand selection algorithm.

Proteins necessary for inflammation, hepatitis and illnesses linked to oxidative stress were thoroughly examined in this docking study. The various protein targets include cyclooxygenase-2 (PDB ID: 3ln0), hepatitis B virus X-interacting protein-HBXIP (pdb:3msh) and superoxide dismutase (PDB: 1e9q).

First, the 3D structures of the target proteins used in this assay were retrieved from the protein data bank (https: www.rcsb.org/) and were subsequently prepared using BIOVIA Discovery Studio Visualizer (BIOVIA 2025). Multiple chains, heteroatoms, energy reduction, shape optimization, and the inclusion of polar hydrogens were all part of the protein preparation process.

The 2D structures of the synthesized compounds were drawn using ChemDraw Professional 15.0 and were converted to their 3D structure using Chem3D.

The synthesized compounds under investigation were docked into the active sites of the target proteins using Autodock Vina Tool (Trott *et al.,* 2010).

Docking results were carefully analyzed with the help of PyMOL and Biovia Discovery Studio Visualizer (BIOVIA 2025), and it was noticed that good interactions like hydrogen

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bonding, van der Waal forces, hydrophobic, alkyl and electrostatic interactions occurred between the studied ligands and proteins.

➢ *In Silico Physicochemical Parameters*

The drug-likeness score of the synthesized compounds was evaluated using SwissADME. In this study, the newly synthesized compounds were drawn using ChemDraw Professional 15.0 and were subsequently converted into SMILES format, and then uploaded directly into the online software tools for molecular properties estimation. The results generated were analyzed using Lipinski's rule of five.

III. RESULTS

➢ *Standard Drug Used:*

Anti-inflammatory (indomethacin), Antioxidant (Vitamin C), Antihepatitic (Silymarin).

Table 1 Binding Energies of the Studied Compounds with the Target Proteins.

S/N	Compounds	Binding affinity (Kcal/mol) Anti-inflammatory target (PDB ID: 3ln0)	Binding affinity (Kcal/mol) Antioxidant target (PDB ID: 1e9q).	Binding affinity (Kcal/mol) Antihepatitic target (PDB ID: 3msh)
1	XY1	-8.5	-6.9	-7.0
2	XY2	-5.8	-3.9	-4.9
3	XY3	-7.0	-5.0	-5.5
4	XY4	-7.9	-4.3	-4.5
5	XY5	-6.1	-4.2	-4.7
	Standard drug	-7.3	-5.1	-8.6

➢ *Types of Interactions Obtained with the Molecules and Target Protein*

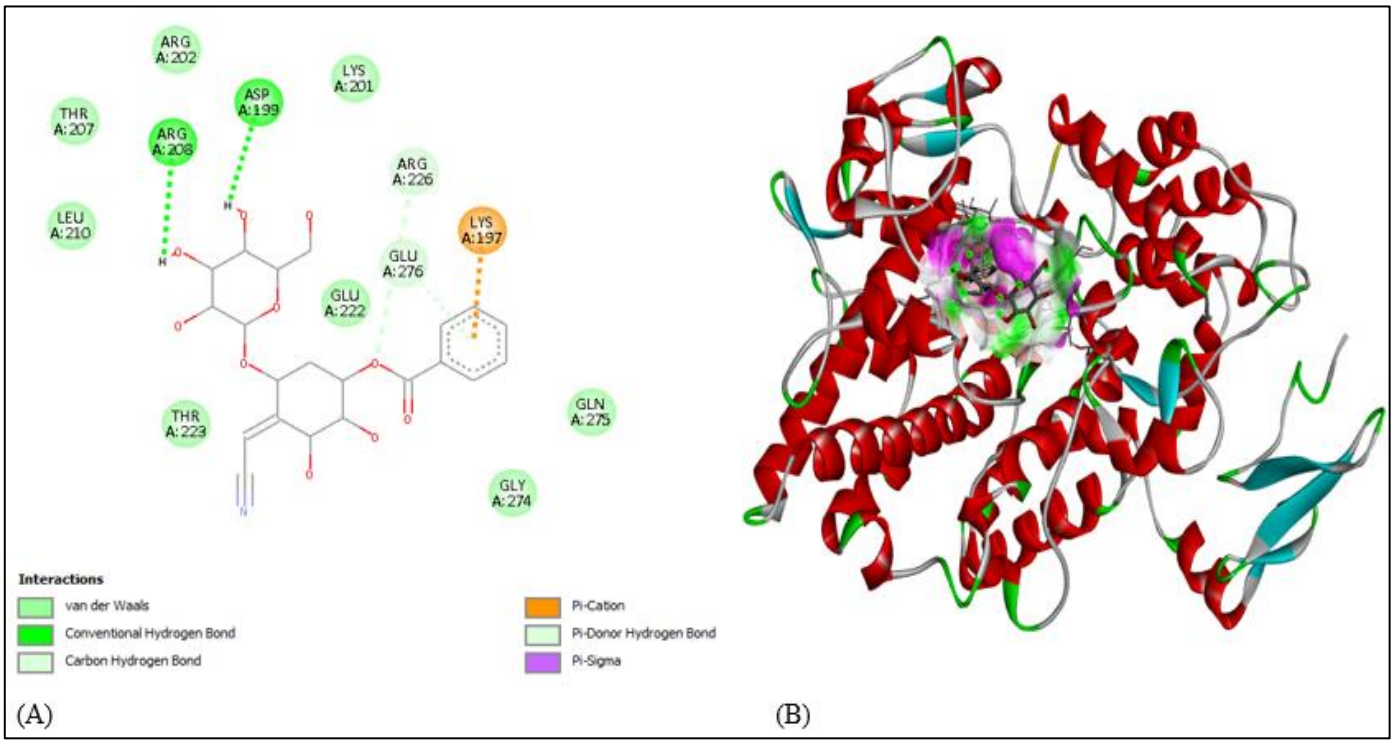

Fig 1 (A) 2D Binding Interactions of Compound XY1 with the Active Site of Cyclooxygenase-2 (COX-2) (PDB ID: 3ln0). (B) 3D Docking Pose of the Ligand in the Pocket Region of the Protein

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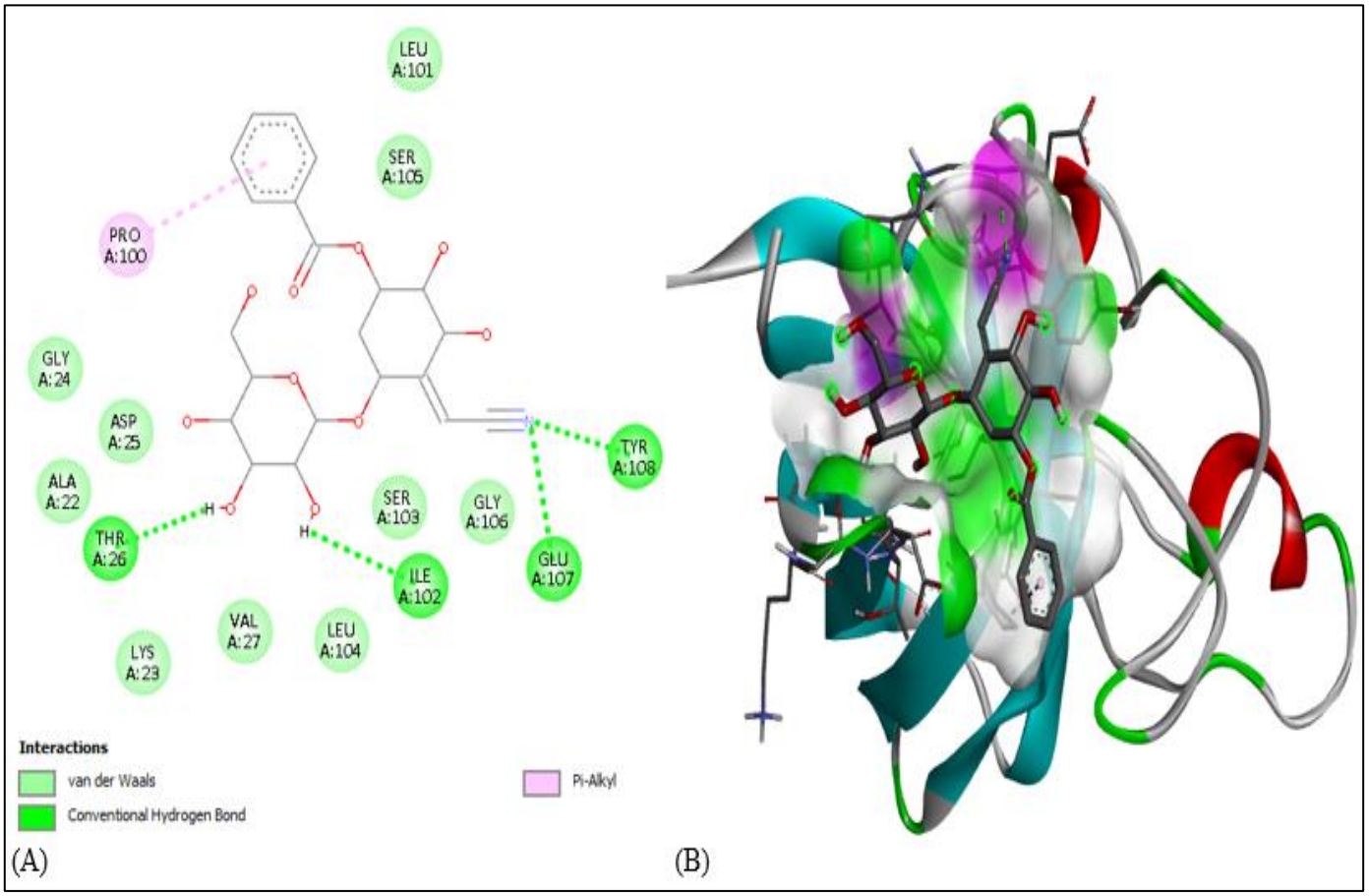

Fig 2 (A) 2D Binding Interactions of Compound XY1 with the Active Site of Superoxide Dismutase (PDB ID: 1e9q). (B) 3D Docking Pose of the Ligand in the Pocket Region of the Protein

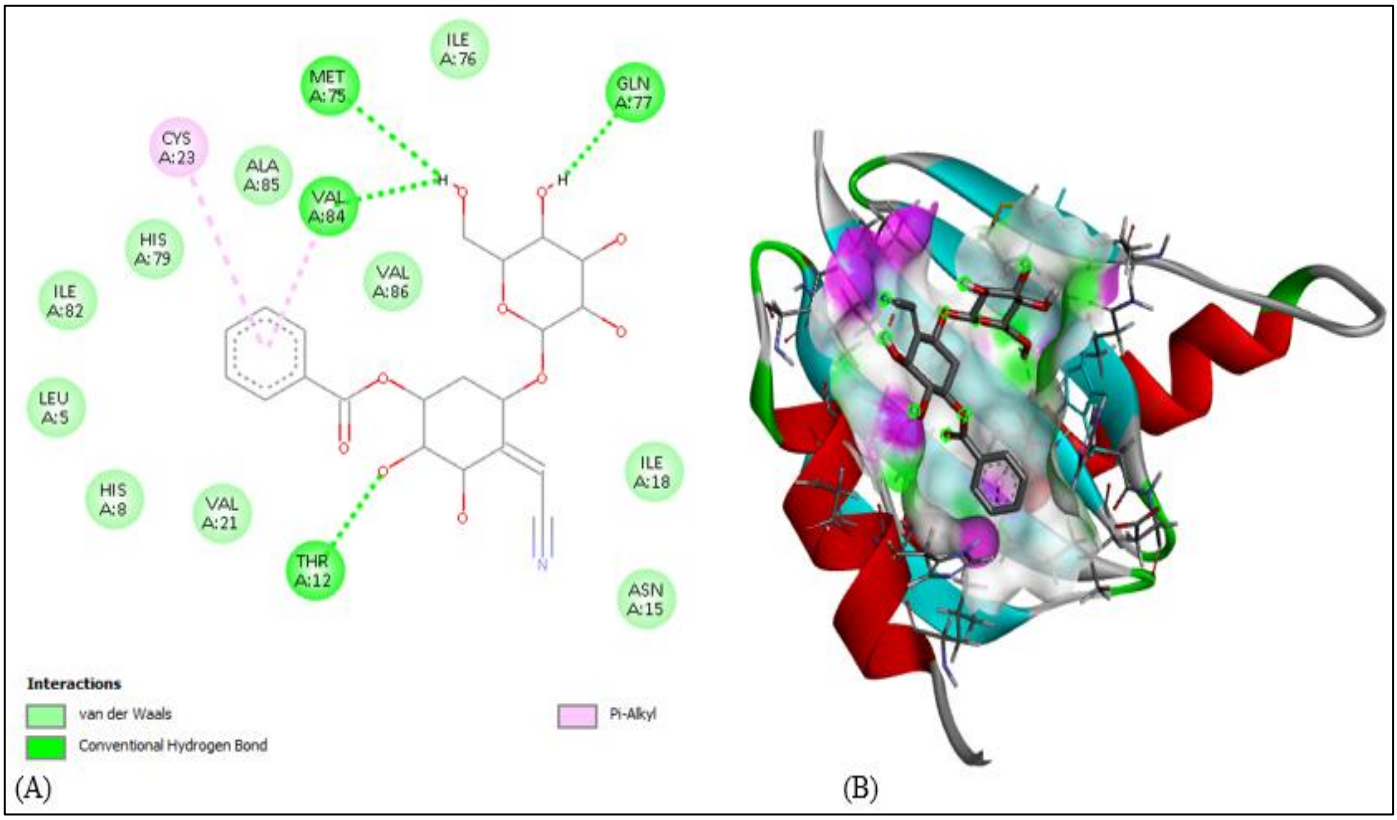

Fig 3 (A) 2D Binding Interactions of Compound XY1 with the Active Site of Hepatitis B Virus X-Interacting Protein-HBXIP (pdb:3msh). (B) 3D Docking Pose of the Ligand in the Pocket Region of the Protein

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➢ *Drug-Like Profile of the Compounds:*

Table 2 Physicochemical properties of the studied compounds (XY1-XY5)

Compounds	MW	tPSA [Å²]	Log P	HBA	HBD	n-RB	Violations
XY1	451.42	189.93	-2.09	11	6	6	3
XY2	268.48	17.07	4.79	1	0	15	1
XY3	206.32	20.23	3.87	1	1	2	0
XY4	652.94	119.36	4.64	8	2	34	2
XY5	296.49	26.30	4.80	2	0	16	1
Lipinski Rule of Five	≤500	≤140	≤5	≤10	≤5	≤10	≤1

- *Abbreviations: MW-*

Molecular weight of the molecule, HBD – predicted number of hydrogen bonds that the solute in an aqueous solution would donate to the water molecules, HBD-estimated number of hydrogen bonds that the solute in an aqueous solution would accept from water molecules, Log P-partition coefficient, n-RB - approximated number of rotatable bonds, tPSA- topological polar surface area. In today's drug development techniques, researchers pay close attention to bioavailability study in order to detect the ability of a potential drug candidate to be orally bioavailable to boycott waste of time, resources and energy. Prior to this, Lipinski's rule of five helps to evaluate the bioavailability for oral drug formulation. This rule highlights certain criteria, called the 'rule of five' which states that an oral drug with a good bioavailability must possess the following: a molecular weight less than 500-daltons, lipophilicity (Log *P*) less than 5, hydrogen bond acceptor less than 10, hydrogen bond donor less than 5. A violation of more than two criteria may result to poor bioavailability. Evidence from Table 2 data shows that only XY1 and XY4 violated the rule with compound XY1 having a tPSA greater than 140A°², hydrogen bond acceptor greater than 10 and hydrogen bond donor greater than 5 while XY4 has a molecular weight of more than 500-daltons and number of rotatable bond greater than 10. Interestingly, the other compounds agree with the Lipinski's rule of five. In addition, tPSA reflects the hydrophilicity of a drug candidate, and it is important in protein-ligand interaction. tPSA for XY2, XY3, XY4 and XY5 reported here in this research is less than 140A°² which is a clear indication that the compounds show high possibility of being a good oral drug candidate.

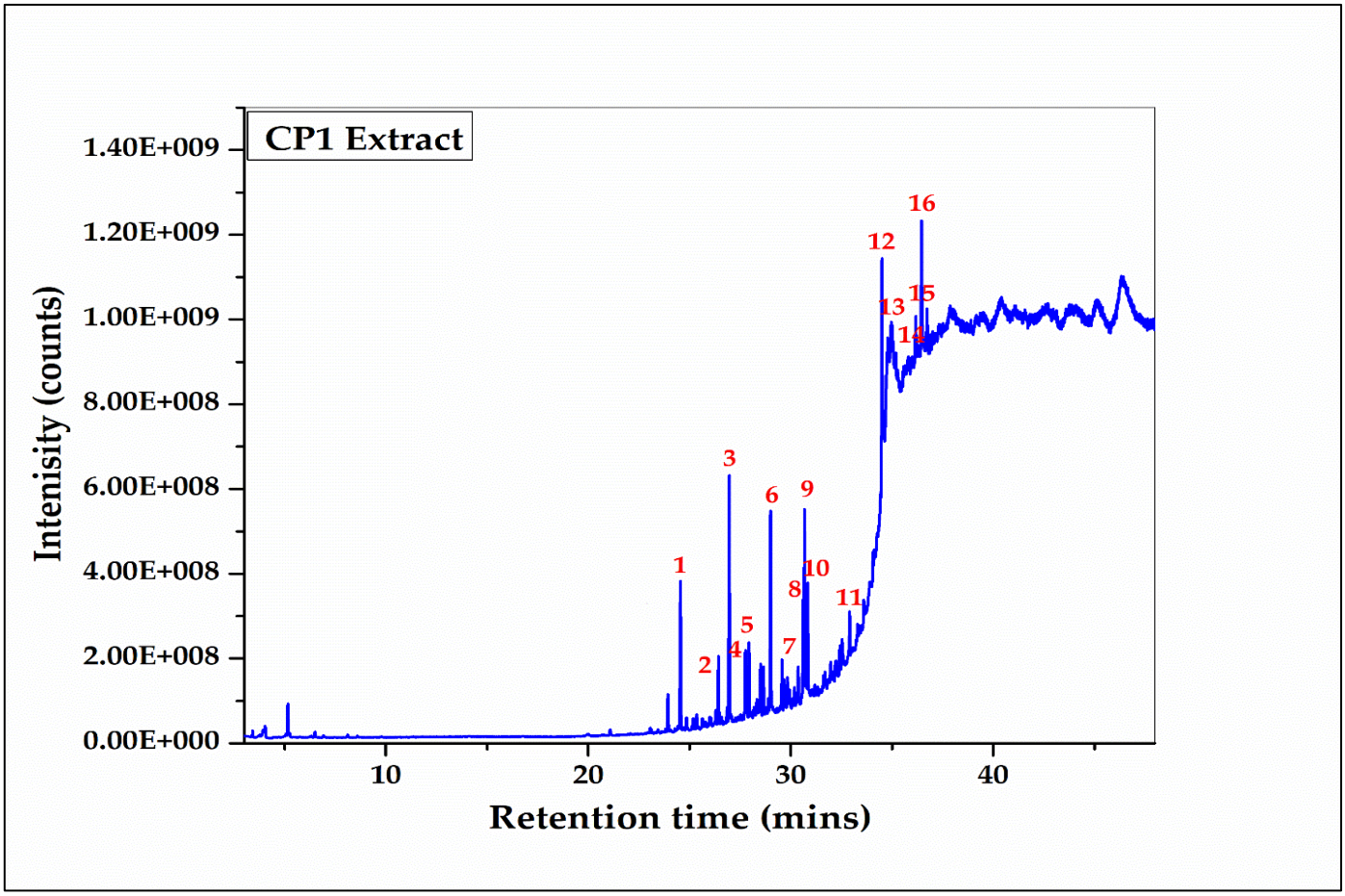

Fig 4 GC-MS of Compounds of the Extract of *L. lanceolata* (CP1)

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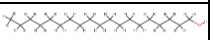
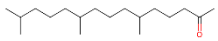
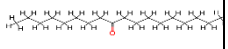
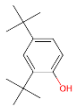
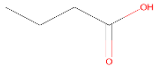
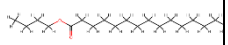
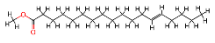
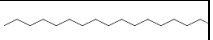
Table 3 GCMS Profile of Major Compounds in the Sample of the Extract of *L. lanceolata* Leaf

S/N	Rt/Mol. Wt	Compound Name	Chemical Formula	% Peak area	Nature	Medical Importance	Reference (s)	Structures
1	24.54/294	10-Heneicosene (c, t)	$C_{21}H_{42}O$	2.90	Hydrocarbon	Potential insecticidal/repellent	Eigenbrode and Espelie (1995)	
2	26.42/282	Eicosane	$C_{20}H_{42}$	1.43	Hydrocarbon	Antimicrobial, anti-cancer, skin conditioning	Satyanarayana & Narasimha (2014); Yang *et al.* (2018)	
3	26.95/284	n-Nonadecanol-1	$C_{19}H_{40}O$	4.56	Fatty Alcohol	Emollient, anti-irritant, membrane-stabilizing effect	Lin *et al.* (2013)	
4	27.75/268	2-Pentadecanone, 6,10,14-trimethyl-	$C_{18}H_{36}O$	1.32	Aliphatic Ketone	Insecticidal, antibacterial, anti-inflammatory	Kim *et al.* (2020); Vining (2018)	
5	27.93/268	9-Octadecanone	$C_{18}H_{36}O$	1.32	Aliphatic Ketone	Insecticidal, antibacterial, anti-inflammatory	Kim *et al.* (2020); Vining (2018)	
6	28.99/406	Nonacos-1-ene	$C_{29}H_{58}$	3.89	Hydrocarbon	Potential insecticidal/repellent	Eigenbrode and Espelie (1995)	
7	29.59/206	2,4-Di-tert-butylphenol	$C_{14}H_{22}O$	0.70	Phenol	Antioxidant, hepatoprotective, neuroprotective, anti-cancer	Lin & Xiao (2019); Sroka & Cisowski (2016)	
8	30.60/398	Benzoic Acid	$C_7H_6O_2$	2.21	Carboxylic Acid	Antimicrobial, preservative, anti-inflammatory	Pinho *et al.* (2018)	
9	30.68/312	Hexadecenoic acid, butyl ester	$C_{20}H_{40}O_2$	3.52	Fatty Acid Esters (Lipids)	Anti-inflammatory, antioxidant, antimicrobial, hypolipidemic	Kumar and Roy (2021); Kato and Watanabe (2018)	
10	30.76/294	Trans-13-Octadecenoic acid, methyl ester	$C_{19}H_{36}O_2$	0.99	Fatty Acid Esters (Lipids)	Anti-inflammatory, antioxidant, antimicrobial, hypolipidemic	Kumar and Roy (2021); Kato and Watanabe (2018)	
11	31.96/242	1-Hexadecanol	$C_{16}H_{34}O$	0.57	Fatty Alcohol	Emollient, anti-irritant, membrane stabilizing effect	Lin *et al.* (2013)	

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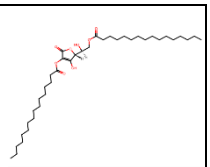
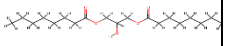
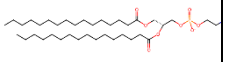
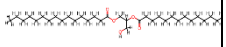
12	34.50/652	l-(+)-Ascorbic acid 2,6-dihexadecanoate	$C_{38}H_{68}O_8$	5.25	Vitamin Esters	Antioxidant, anti-aging, immunomodulatory	Padayatty & Levine (2016); Das & Das (2017)	
13	34.87/344	1,3-Dioctanoin	$C_{19}H_{36}O_5$	3.85	Glycerides/Phospholipids	Energy supplementation, prebiotics, and antimicrobial.	Nagao and Yanagita (2005	
14	34.95/692	Hexadecenoic acid, 1-[[[(2-aminoethoxy) hydroxyphosphinyl] oxy] methyl]-1,2-ethanediyl ester	C37H74NO8P	2.97	Glycerides/Phospholipids	Potential immunomodulatory, structure role in cell membranes	Guschina and Harwood (2006)	
15	35.18/568	Hexadecenoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	$C_{35}H_{68}O_5$	2.17	Glycerides/Phospholipids	Potential antimicrobial and surfactant-like properties	Guschina and Harwood (2006)	
16	36.46/282	cis-Vaccenic acid	$C_{18}H_{34}O_2$	2.82	Fatty acid	Modulation of lipid metabolism, cardioprotective, anti-inflammatory	Yang *et al.* (2017)	

IV. DISCUSSION

Molecular docking study was carried out to ascertain the inhibitory activities of the studied compounds against three enzymes. The result of the binding energies of the compounds (XY1-XY5) against the target receptors are reported in Table 1. Base on the anti-inflammatory docking assay as presented in Table 1, XY1 and XY4 are hit compounds which had a better binding affinity of -8.5 Kcal/mol and -7.9 Kcal/mol compared to the clinical drug, indomethacin with a binding affinity of -7.3 Kcal/mol. XY3 showed a good binding energy of -7.0 Kcal/mol which is slightly comparable to that of indomethacin at -7.3 Kcal/mol.

In-silico molecular docking antioxidant activities of the studied compounds against the studied enzyme reveals that only XY1 had a better activity than the standard drug, Vitamin C. XY3 showed a good binding energy of -5.0 Kcal/mol comparable to Vitamin C, a clinical drug currently available in clinics.

Antihepatitic molecular docking research shows that all the studied compounds had a smaller binding energy than Silymarin, a standard drug currently used in the management of hepatitis. XY1 with a good binding energy of -7.0 Kcal/mol was the only compound which showed appreciable inhibition properties against the target enzyme compared to Silymarin with a binding energy of -8.6 Kcal/mol.

The molecular docking studies show that XY1 can act as a good anti-inflammatory, antioxidant and antihepatitic inhibitors at different targets.

It was observed that the studied compounds were able to interact with each of the anti-inflammatory, antioxidant and antihepatitic target proteins, inhibiting their biochemical processes with XY1 showing highest binding energies across the three different proteins, thus it is considered a hit compound for further investigation. As represented in figure 1, there exist a favorable hydrogen bond interaction between ARG 208 and ASP 199 while other interactions were noticed with pi-cation and van der waal's interaction.

V. CONCLUSION

In conclusion, the compounds from the natural product were evaluated as antioxidants, anti-inflammatory, antihepatitic and hepatoprotective therapeutics against liver disorders. From docked compounds, we propose for the first time that the studied compounds; cis-vaccenic acid, L-(+)-ascorbic acid 2,6-dihexadecanoate, hexadecenoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester, 2,4-Di-tert-btylphenol demonstrated high binding affinity than silymarin for treatment of hepatitis. Further studies must be conducted to ascertain the detailed mechanistic and antiviral efficacy of the analyzed compounds.

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