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GC-MS and Molecular Docking Analyses of Phytoconstituents from the Plant Tephrosia purpurea

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KEYWORDS

Tephrosia purpurea, GC-MS, Molecular docking, Anti-inflammatory

ABSTRACT:

Introduction: Medicinal plants are extremely useful assets in the development of novel medications and plant-derived treatments. The use of herbs in the treatment of chronic and acute diseases, as well as a wide range of ailments and issues, including cardiovascular disease, depression, inflammation, and other conditions. According to the prior ethnobotanical study, Tephrosia purpurea has healing capabilities for external wounds, kidneys, liver, spleen, and blood-related disorders.

Objectives: This study aimed to explore the phytochemical present in the plant extract of Tephrosia purpurea and the binding affinity of the anti-inflammatory activity of that compound by the In-silico molecular docking method.

Methods: A continuous hot extraction process was performed on 100 grams of shade-dried coarse powder obtained from the aerial part. The analysis using Agilent 5977 MSD technology was performed for GC-MS. Molecular docking was performed utilizing the phytochemicals found from the gas chromatography-mass spectrometry (GC-MS) study of TPP and TPE. The protein structures used for molecular docking include cyclooxygenase-2, 5-Lipoxygenase, PDE4, and Human peroxiredoxin 5.

Results: GC-MS analysis of TP petroleum ether extract identified 10 phytoconstituents among these four compounds were major compounds.; 9,12,15-Octadecatrienoic acid, (Z, Z, Z)- (41.79); n-Hexadecanoic acid (39.74); Phytol (9.03); and 2-Benzoylamino-3-(p-tolyl-)-N, N-dimethyl-propenamide (3.22). GC-MS ethanolic extract of TP revealed 11 phytoconstituents and from these four major components; Trimethylsilyl (5E,13E)-9,11,15-tris[(trimethylsilyl) oxy] prosta-5,13-dien-1-oate # (65.24); Phytol (23.38); 25-Norisopropyl-9,19-cyclolanostan-22- en-24-one,3-acetoxy-24-phenyl-4,4,14- trimethyl (5.54); Pregnane-12,18,20-triol, 18,20-isopropylidene-3,3-ethylenedioxy (2.19). The docking score analysis indicated that all ligands exhibited activity within a range of -4.5 to -16.2 kcal/mol against Cox-2, -4.4 to -13.5 kcal/mol against 5LOX, -3.7 to -16.3 kcal/mol against PDE4, and -3.6 to -12.1 kcal/mol against HP5. The compounds Pregnane-12,18,20-triol, 18,20-isopropylidene-3,3-ethylenedioxy; 25-Norisopropyl-9,19-cyclolanostan-22-en-24-one,3-acetoxy-24-phenyl-4,4,14-trimethyl; and 7,8,12-Tri-O-acetyl-3-desoxy-ingol-3-one have possessed highest docking score against the protein Cox-2, 5LOX, PDE4, and HP5.

Conclusions: The plant might serve to make drugs that are useful for a wide range of diseases. To figure out what biological effects it has, more study is needed.

1. Introduction

Medicinal plants are invaluable resources when it comes to developing new pharmaceuticals and plant-based remedies. Most natural chemicals are bioactive molecules from animals, plants, and microbes. They are vital repositories for novel pharmacological compounds, medicinal precursors, and unique chemical compound entities, advancing human civilization [37]. Utilizing herbal medicine as an alternate form of medical treatment. Due to their growing traditional usage and cultural acceptance, these medicinal herbs are highly esteemed and have few adverse effects, making them more significant on a global scale [53]. Worldwide investigations have been conducted to confirm the effectiveness of plant-based medications, and some of the results have resulted in the development of these

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medicines in modern times. The annual global demand for medicinal plant products surpasses $100 billion [49]. Furthermore, the therapeutic efficacy and chemical constituents of certain medicinal plant species remain undisclosed. Therefore, further research is necessary to uncover new phytoconstituents and explore the biological activity of these plant species. New drug discovery begins with natural active principal identification. Plant extract screening is a new way to uncover beneficial compounds in different plant species. Phenolic, flavonoids, alkaloids, tannins, saponins, and terpenoids are among the phytochemicals that possess a variety of biological activities, including anti-inflammatory, antioxidant, anti-ulcer, anti-diarrhea, and anticancer properties [42].

Spectrometric and chromatographic screenings of medicinal plants yield useful data about their chemical and pharmacological properties, which aids in the selection of plants with biological activity [30]. Gas chromatography-mass spectrometry (GC-MS) is a very effective, rapid, and precise method for identifying a wide range of substances, such as alkaloids, alcohols, organic acids, long-chain hydrocarbons, nitro compounds, steroids, esters, and amino acids [35].

Cyclooxygenase-2 (COX-2) is a significant contributor to tissue inflammation due to its involvement in the formation of Prostanoids. It achieves this by metabolizing arachidonic acid into prostaglandin H (PGH) [10]. Lipoxygenases (LOX) catalyze the synthesis of leukotrienes via a series of enzymatic processes. Leukotrienes, including leukotriene B4 (LTB4) and cysteinyl leukotrienes (LTC4, LTD4, and LTE4), exert a substantial influence on several inflammatory mechanisms. LTB4 is a potent chemotactic agent that attracts immune cells, specifically neutrophils, to areas of inflammation. The cysteinyl leukotrienes play a crucial role in disorders such as asthma and allergic rhinitis by causing increased vascular permeability, bronchoconstriction, and mucus secretion. Therefore, 5-LOX inhibitors are the preferred anti-inflammatory medications for people with asthma [25]. The phosphodiesterase enzyme plays a crucial role in cellular signaling by breaking down and degrading cyclic AMP (cAMP) and cyclic GMP (cGMP) [4]. Elevated levels of cAMP and cGMP in the smooth muscles of the arteries lead to decreased calcium levels, resulting in the reduction of vascular contraction. Decreased vascular constriction results in the widening of blood vessels, decreased aggregating of platelets, and reduced levels of interleukin [38]. Human Peroxiredoxin (HP5) functions as an antioxidant and plays a crucial role in the cellular response to oxidative stress. The oxidation of amino acids results in the impairment of enzymes' active sites, which in turn leads to structural damage to proteins, causing significant disruption to the protein mechanism. Peroxiredoxin 5 functions by removing peroxides and restricting the production and release of inflammatory mediators. Gaining a comprehensive understanding of the mechanisms and control of these enzymes is essential to devise appropriate treatment approaches for the management of inflammation and associated diseases [15].

Tephrosia purpurea (TP) belonging to the family Fabaceae is a perennial plant that grows upright or spreads horizontally, reaching a maximum height of 50-60 m. The plant contains a variety of traditional therapeutic uses, as it is collected from its natural habitat [31]. The previous ethnobotanical survey has claimed that it exhibits curative properties for external wounds, kidneys, liver, spleen, and diseases related to the blood. The dried herbs have many medicinal uses, including as a diuretic and tonic laxative; they are also applied topically to treat conditions such as bilious fever attacks, boils, pimples, bleeding piles, and bronchitis [12]. The infusion of Tephrosia purpurea is employed for oral washing [51]. The root part of the TP has been used for treating inflammation, skin problems, elephantiasis, flatulence, hemorrhoids, asthma, bronchitis, anemia, dysmenorrhea, chronic fever, boils, pimples, and gingivitis. The leaves part of the TP is employed to treat dyspepsia, pectoral disease, hemorrhoids, syphilis, and gonorrhea. The whole plant has been used for the treatment of tumors, ulcers, and leprosy, as well as allergic and inflammatory conditions like rheumatism, asthma, and bronchitis [12], [16]. A concoction made from crushed leaves of TP is utilized as a remedy for snake bites. In Punjab, the infusion of seeds is regarded as having a cooling effect. In Sri Lanka, a decoction made from the roots is utilized as a nematicide to treat the larvae of Toxocara canis, which is responsible for causing lung disease. In Ceylon, it is utilized as an anthelmintic specifically for children. It is used to treat liver disorders in India. Also used for cirrhosis, hepatitis, bilious febrile episodes, splenic diseases, and the liver.

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The oil extracted from seeds is employed to treat scabies, eczematous irritation, and various skin eruptions. It is also utilized for the treatment of piles, syphilis, and gonorrhea. Additionally, the leaves are used as animal feed in India and South Africa [47]. Previous investigation reported the presence of secondary metabolites of phenolic and flavonoid compounds likewise, Chlorogenic acid, Gallic acid, Methyl gallate, Caffeic acid, Rutin, Pyrocatechol, Ellagic acid, Coumaric acid, Vanillin, Ferulic acid, Naringenin, Quercetin, Kaempferol, Cinnamic acid, Apigenin, Hesperetin. The major compounds identified in the GC-MS analysis of methanol and n-hexane extracts of TP are stigmasta5,24(28)-dien-3-ol, (3β,24Z)- (44.74%) and 9,12,15-octadecatrienoic acid methyl ester (0.67%) [52]. In other studies, identified chemical constituents like; Dried fruits include compounds, including lanceolatin B, (+) purpurin, O-methylpongamol, and maackiain [32]. Flowers include compounds such as Delphinidin chloride, cyaniding, karanjin, and kanjon [32]. Leaves comprise Lupeol, Rutin, Rotenoid, triterpenoid, and beta-sitosterol [34]. Pods and seeds contain the compounds purpurin, purpuritenin A, purpuritenin B, tephroglabrin, tepurinidiol, purpureamethide, O-methylpongamol, sitosterol [32], rotenoid, diketone-pongamol, isolonchocarpin, furanoflavones karanjin and kanjone, and flavanone purpurin. Seeds also contain a flavonoid called lanceolarin B [34]. The root contains the following compounds purpurenone, purpurin, dehydroisoderricin, maackiain, new epoxflavanone, pongamol, flemichapparins B and C, rutin, methylkaranjic acid, sitosterol, spinasterol, lanceolatin A, and lanceolatin B [32]. The stem consists of 7-0-[beta-D-glucopyranosyl-(1-4)-0-BETA-D-galactopyranosidel [31]. Tephrosin, pongaglabol, and semiglabrin are present in the aerial parts [3]. Several pharmacological activities have been associated with Tephrosia purpurea, including anti-allergic [19], potent membrane stabilizing [18], renal protective [33], antiulcer [14], hepatoprotective [28], anti-inflammatory, and analgesic effects [20], antioxidant [46], anthelmintic [45], antibacterial [1], antiviral [43], anti-diarrheal [29], anticancer [21], anti-epileptic [8], and anti-hyperglycemic [44]. This study aims to analyze the bioactive compounds found in Tephrosia purpurea using the GC-MS method. Additionally, it aims to determine the binding affinity of these compounds with Cox-2, 5LOX, PDE4, and HP5.

2. Materials and methods

Collection, processing, and extraction

The fresh aerial part of Tephrosia purpurea (TP) was collected from an adjoining area of Barpali (Dist. Bargarh, Odisha) in July. The plant was authenticated by Mr. S. N. Badapanda, Botanist Sriram College, Rampur.

Preparation of plant extract

The aerial part was dried under shade and powdered with the help of a mechanical grinder. The coarse powder is stored in an airtight container for further studies. The shade-dried coarse powder of the aerial part (100 g) was subjected to continuous hot extraction with the solvent petroleum ether (60–80o C), and ethanol as per their polarity successively. The extraction process was carried out until all dissolved components were eluted, taking into account the boiling point of the solvents. The extracts were concentrated using a rotary evaporator and kept cool in a desiccator.

Gas chromatography-mass spectrometry (GC-MS) analysis

GC-MS analysis was carried out in Agilent 5977 MSD technology. The mass-spectrophotometer, fitted with anHP-5 MS fused silica column (Dimensions 30 m x 250 µm x 0.25 µm), interfaced with MSD. The carrier gas was used as Helium and the velocity flow of the column was adjusted to 1.2ml/min. The temperature of the column ranged from 600C - 3250C (3500C) and the pressure was 11.367psi. The total run time of GC was 41.5 minutes. 1 µl of sample was injected through the injector and the mass was taken at 70eV. The quad temperature was set at 1500C and the source temperature was set at 2300C for up to 10 minutes holding time. [13].

In-Silico Molecular Docking

Molecular docking was conducted using the phyto-constituents identified from GC-MS analysis of TPP and TPE. The 3D crystal structures of cyclooxygenase-2 (PDB ID: 3mdl), 5-Lipoxygenase (PDB ID: 6ncf), PDE4 (PDB ID: 4wcu), and Human peroxiredoxin 5 (PDB ID: 1hd2) were obtained from the protein data bank. The 3D structure of Indomethacin (PubChem CID: 3715); Docosahexaenoic acid, 1,2,3-propanetriyl ester

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(PubChem CID 9546569); 10,13-Eicosadienoic acid, methyl ester (PubChem CID 5365687); Docosanoic acid nonyl ester (PubChem CID 537333); 2-Tridecanone (PubChem CID 11622); Pentacosanoic acid, methyl ester (PubChem CID 41431); n-Hexadecanoic acid (PubChem CID 985); Phytol (PubChem CID 5280435); 9,12,15-Octadecatrienoic acid, (Z, Z, Z)- (PubChem CID 5280934); 2-Benzoylamino-3-(p-tolyl-)-N, N-dimethyl-propenamide (PubChem CID 5369671); psi.,. psi. -Carotene, 7,7',8,8',11,11',12,12',15,15'-decahydro (PubChem CID 5365816); Trimethylsilyl (5E,13E)-9,11,15-tris[(trimethylsilyl) oxy] prosta-5,13-dien-1-oate # (PubChem CID 5366438); Docosanoic acid, 1,2,3-propanetriyl ester (PubChem CID 62726); Pregnane-12,18,20-triol, 18,20-isopropylidene-3,3-ethylenedioxy (PubChem CID 567464); Demeclocycline (PubChem CID 54680690); Hyocholic acid (PubChem CID 92805); Xanthophyll (PubChem CID 5281243); 4a-Phorbol 12,13-didecanoate (PubChem CID 452544); Octadecane, 1,1'-[1,3-propanediylbis(oxy)] bis (PubChem CID 624534); 25-Norisopropyl-9,19-cyclolanostan-22- en-24-one,3-acetoxy-24-phenyl-4,4,14- trimethyl (PubChem CID 5373661); 7,8,12-Tri-O-acetyl-3-desoxy-ingol-3-one (PubChem CID 541413) were taken from PubChem. The protein was prepared by using AutoDock tools-1.5.7, and the crystallographic structure chain A was used for the docking process [39]. To identify the active site, the water molecules and co-crystal ligands were eliminated, polar hydrogen was added, and the Kollman charge was then applied. To prepare the ligands, Open Babel software (v.2.4.1) was used [40]. Active areas were defined as those parts of amino acids that were shown to interact with the ligands listed in the protein files. The grid box was set with dimensions of 60×60×60 points for Cox-2, 5LOX, PDE4, and 40×40×40 points for HP5 in the x, y, and z directions. The grid centers for Cox-2, 5LOX, PDE4, and HP5 were located at coordinates (25.924, 21.223, 65.974), (24.889, -22.451, 33.681), (19.048, -11.068, -4.778), and (8.009, 42.610, 20.044) respectively. The docking was performed by using AutoDock Vina software for docking score and 3D visualization was performed with Biovia Discovery Studio 2021 Client.

3. Results & discussion

GC-MS analysis of Tephrosia purpurea

GC-MS chromatogram of petroleum ether extract of Tephrosia purpurea (TPP) and ethanol extract of Tephrosia purpurea (TPE) were presented in Figures (1, and 3). The retention time (Rt), Name of the compound, nature of the compound, molecular formula, molecular weight, peak area %, and biological activity of the respective compounds were represented in Tables (1 and 2). The structure of the phytocompounds was depicted in Figures (2, and 4). GC-MS analysis of TP petroleum ether extract identified 10 phytoconstituents among these four compounds were major compounds.; 9,12,15-Octadecatrienoic acid, (Z, Z, Z)- (41.79); n-Hexadecanoic acid (39.74); Phytol (9.03); and 2-Benzoylamino-3-(p-tolyl-)-N, N-dimethyl-propenamide (3.22). The rest compounds were minor; Docosahexaenoic acid, 1,2,3-propanetriyl ester (1.47); and psi.,. psi. -Carotene, 7,7',8,8',11,11',12,12',15,15'-decahydro (1.34); Docosanoic acid nonyl ester (1.18); 10,13-Eicosadienoic acid, methyl ester (0.89); 2-Tridecanone (0.76); Pentacosanoic acid, methyl ester (0.57). GC-MS ethanolic extract of TP revealed 11 phytoconstituents and from these four major components; Trimethylsilyl (5E,13E)-9,11,15-tris[(trimethylsilyl) oxy] prosta-5,13-dien-1-oate # (65.24); Phytol (23.38); 25-Norisopropyl-9,19-cyclolanostan-22- en-24-one,3-acetoxy-24-phenyl-4,4,14- trimethyl (5.54); Pregnane-12,18,20-triol, 18,20-isopropylidene-3,3-ethylenedioxy (2.19). The rest compounds were minor Octadecane, 1,1'-[1,3-propanediylbis(oxy)] bis (1.10); Docosanoic acid, 1,2,3-propanetriyl ester (0.98); 7,8,12-Tri-O-acetyl-3-desoxy-ingol-3-one (0.54); Xanthophyll (0.47); 4a-Phorbol 12,13-didecanoate (0.32); Hyocholic acid (0.20); Demeclocycline (0.02).

Gas chromatography-mass spectrometry (GC-MS), an effective method for phytoconstituent separation, was employed to conduct the analysis [35]. GC-MS study on the petroleum ether and ethanol extract of TP identified the phytoconstituents that may be responsible for the therapeutic benefits of this plant species. The compounds from petroleum ether extract of TP, Docosahexaenoic acid, and 1,2,3-propanetriyl ester a triglyceride in nature and possess Anti-oxidant, Hypocholesterolemic,

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nematicide, pesticide, lubricant, and Anti-androgenic activity [17]. 10,13-Eicosadienoic acid, methyl ester has been reported for antimicrobial activities [22]. The fatty acid compound Docosanoic acid nonyl ester exhibited arachidonic acid inhibitors, urinary acidulants, and urine acidifier activities. 2-Tridecanone which has methyl ketone compound with Insecticidal activity [11]. n-Hexadecanoic acid which is a long-chain fatty acid and one of the major compounds identified in petroleum ether extract exhibited antioxidants, hypocholesterolemic, nematicide, pesticide, and anti-inflammatory activity [48], [7]. The diterpenoid compound phytol revealed Anxiolytic, cytotoxic, antioxidant, autophagy, apoptosis-inducing, antinociceptive, anti-inflammatory, immune-modulating, and antibacterial activities [27]. 9,12,15-Octadecatrienoic acid, (Z, Z, Z)- has shown Antiarthritic, Anticancer, Hepatoprotective, Antimicrobial, and Antiasthma activity [36]. psi.,. psi. -Carotene, 7,7',8,8',11,11',12,12',15,15'-decahydro possessed antioxidant activity [5]. The compounds of ethanolic extract of TP revealed various biological activities; Docosanoic acid, 1,2,3-propanetriyl ester have Anti-oxidant, Hypocholesterolemic, nematicide, pesticide, lubricant, Anti-androgenic activities [17]. Pregnane-12,18,20-triol, 18,20-isopropylidene-3,3-ethylenedioxy possessed anti-oxidant activity [23]. Demeclocycline has been shown to have properties like antibiotics and inhibitors of arginine vasopressin [54]. The conjugate acid compound hyocholic acid is a biomarker for metabolic disorders [24]. The Carotenol compound Xanthophyll exhibited anti-cancer properties [50]. 4a-Phorbol 12,13-didecanoate involved direct activation of TRPV4 [6]. Octadecane, 1,1'-[1,3-propanediylbis(oxy)] bis is a Nucleic acid transfer carrier, manufacturing nucleic acid, and it is used for manufacturing nucleic acid [41]. The terpenoids compound 25-Norisopropyl-9,19-cyclolanostan-22- en-24-one,3-acetoxy-24-phenyl-4,4,14- trimethyl possessed Antibacterial and antifungal activity [2]. 7,8,12-Tri-O-acetyl-3-desoxy-ingol-3-one have Antibacterial activity and antioxidant activity [26].

In-Silico Molecular Docking

The docking score analysis revealed that all ligands demonstrated activity ranging from -4.5 to -16.2 kcal/mol against Cox-2, from -4.4 to -13.5 kcal/mol against 5LOX, from -3.7 to -16.3 kcal/mol against PDE4, and from -3.6 to -12.1 kcal/mol against HP5. Phytoconstituents demonstrated superior binding ability against COX-2 and PDE4 compared to the 5LOX and HP5 targets, as indicated by their total docking score. The height docking score of these compounds are Pregnane-12,18,20-triol, 18,20-isopropylidene-3,3-ethylenedioxy (-16.2, -13.5, -16.3, -12.1); 25-Norisopropyl-9,19-cyclolanostan-22- en-24-one,3-acetoxy-24-phenyl-4,4,14- trimethyl (-14.1, -11.8, -14.9, -10.4); and 7,8,12-Tri-O-acetyl-3-desoxy-ingol-3-one (-11.6, -9.7, -12.5, -8.6) against Cox-2, 5LOX, PDE4, and HP5 (Table 3). The hydrogen bond interactions are represented in Table 4 and Figs. 6-13. When compared to other proteins, HP5 was shown to have the highest number of hydrogen bonds formed when ligands interacted with it. The compound 9,12,15-Octadecatrienoic acid, (Z, Z, Z)- interacts with the amino acids LYS63, LYS63, LYS63, VAL70, and LYS93 with bond angles of 2.33593, 2.24278, 2.24278, 2.19502, and 2.19159, respectively. Demeclocycline interacts with the amino acids ASP77, ARG124, ARG124, ARG124, PRO100, ILE119, and ILE119, affecting the bond angles of 2.26896, 3.35565, 2.93055, 2.89081, 2.34588, 2.83606, and 2.87033. Hyocholic acid forms interactions with the amino acids LYS63, VAL70, GLU16, VAL70, ARG86, and VAL69. These interactions involve bond angles of 3.0228, 2.93723, 2.27491, 2.25509, 2.94232, and 3.5198.

Table 01: GC-MS analysis of Petroleum ether extract of *Tephrosia purpurea*

Sl.no.	RT	Name of the compound	Nature of compound	M.F.	M.W. g/mol	Peak % area	Biological activity	Ref.
1	19.08	Docosahexaenoic acid, 1,2,3-propanetriyl ester	Triglyceride	$C_{69}H_{98}O_6$	1023.5	1.47	Anti-oxidant, Hypocholesterolemic, nematicide, pesticide, lubricant, Anti-androgenic activity	[17]

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2	19.6	10,13-Eicosadienoic acid, methyl ester	-	$C_{21}H_{38}O_2$	322.5	0.89	Antimicrobial activity	[22]
3	20.9	Docosanoic acid nonyl ester	Fatty acid	$C_{31}H_{62}O_2$	466.8	1.18	arachidonic acid inhibitors, urinary acidulants, and urine acidifiers	[9]
4	23.7	2-Tridecanone	Methyl ketone	$C_{13}H_{26}O$	198.34	0.76	Insecticidal activity	[11]
5	25.09	Pentacosanoic acid, methyl ester	Fatty acid	$C_{26}H_{52}O_2$	396.7	0.57	Not reported	
6	27.41	n-Hexadecanoic acid	Long chain fatty acid	$C_{16}H_{32}O_2$	256.42	39.74	antioxidants, hypocholesterolemic, nematicide, and pesticide, anti-inflammatory activity.	[48], [7]
7	29	Phytol	Diterpenoid	$C_{20}H_{40}O$	296.5	9.03	Anxiolytic, cytotoxic, antioxidant, autophagy and apoptosis-inducing, antinociceptive, anti-inflammatory, immune-modulating, and antibacterial activities	[27]
8	30.45	9,12,15-Octadecatrienoic acid, (Z, Z, Z)-	Steroid	$C_{18}H_{30}O_2$	278.4	41.79	Antiarthritic, Anticancer, Hepatoprotective, Antimicrobial, Antiasthma	[36]
9	35.56	2-Benzoylamino-3-(p-tolyl-)-N, N-dimethyl-propenamide	-	$C_{19}H_{20}N_2O_2$	308.4	3.22	Not reported	
10	37.54	psi.,. psi. -Carotene, 7,7',8,8',11,11',12,12',15,15'-decahydro	Carotenoid	$C_{40}H_{66}$	547	1.34	Antioxidant	[5]

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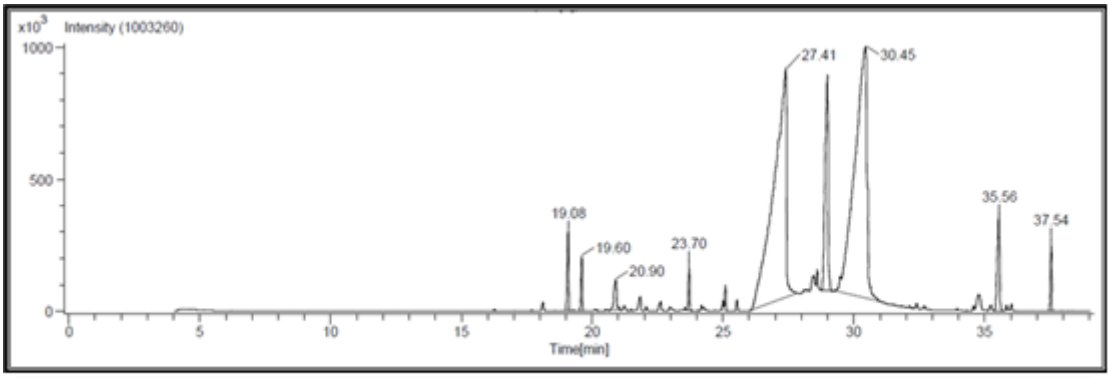

Fig 01: GC-MS chromatogram of the Petroleum ether extract of *Tephrosia purpurea*

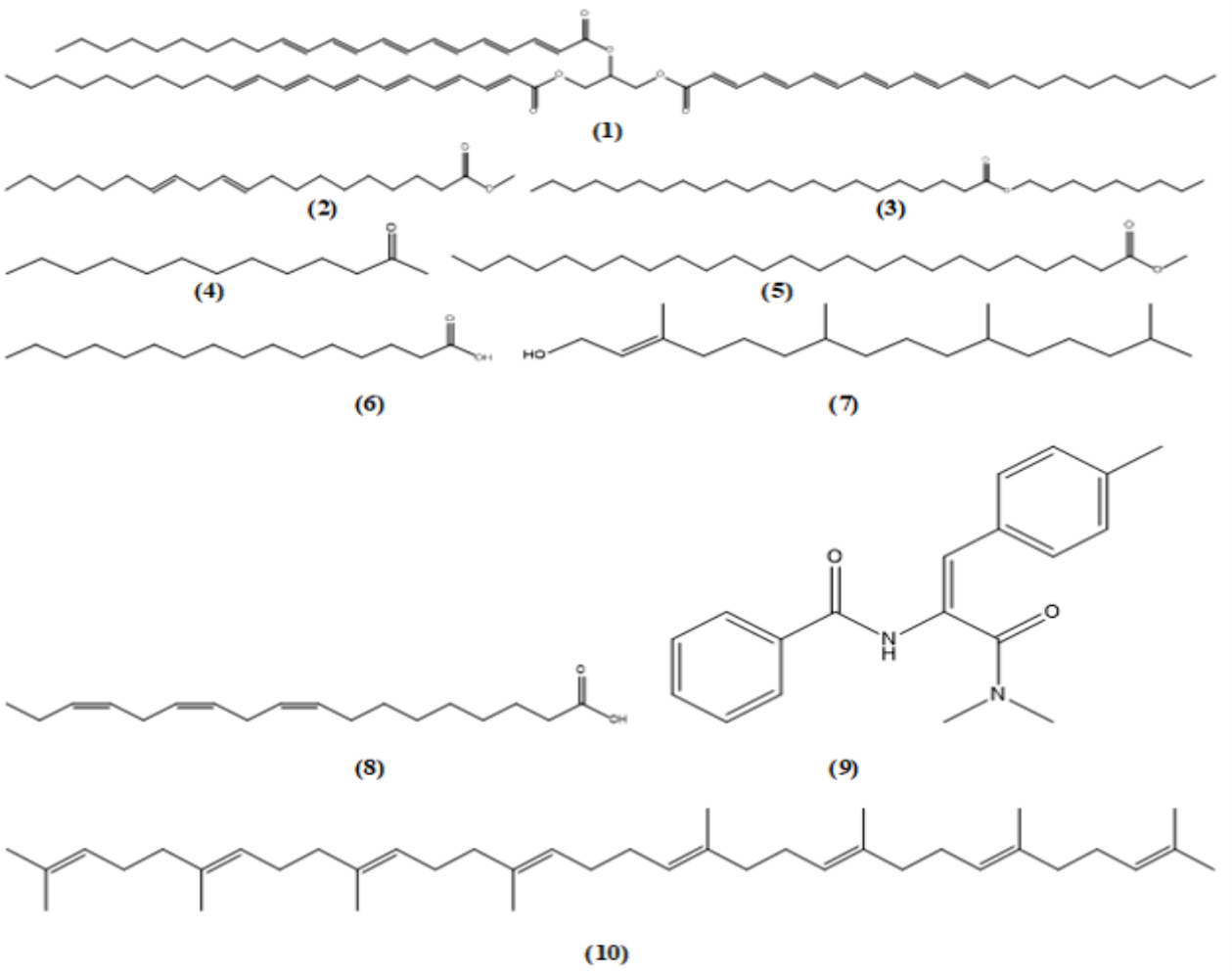

Fig. 02: Structure of compound from GC-MS analysis of Petroleum ether extract of *Tephrosia purpurea*

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Table 02: GC-MS analysis of ethanol extract of *Tephrosia purpurea*

Sl. no.	RT	Name of the compound	Nature of compound	M.F.	M.W. g/mol	Peak % area	Biological activity	Ref.
01	25.74	Trimethylsilyl (5E,13E)-9,11,15-tris[(trimethylsilyl) oxy] prosta-5,13-dien-1-oate #	-	$C_{32}H_{66}O_5Si_4$	643.2	65.24	Not reported	
02	26.24	Docosanoic acid, 1,2,3-propanetriyl ester	-	$C_{69}H_{134}O_6$	1059.8	0.98	Anti-oxidant, Hypocholesterolemic, nematicide, pesticide, lubricant, Anti-androgenic activities	[17]
03	26.46	Pregnane-12,18,20-triol, 18,20-isopropylidene-3,3-ethylenedioxy	-	$C_{26}H_{42}O_5$	434.6	2.19	Anti-oxidant activity	[23]
04	28.81	Phytol	Diterpenoid	$C_{20}H_{40}O$	296.5	23.38	Anxiolytic, cytotoxic, antioxidant, autophagy and apoptosis-inducing, antinociceptive, anti-inflammatory, immune-modulating, and antibacterial activities	[27]
05	29.46	Demeclocycline	-	$C_{21}H_{21}ClN_2O_8$	464.86	0.02	Antibiotic, inhibitor of arginine vasopressin	[54]
06	29.53	Hyocholic acid	Conjugate acid	$C_{24}H_{40}O_5$	408.6	0.20	Biomarker for metabolic disorders	[24]
07	29.65	Xanthophyll	Carotenol	$C_{40}H_{56}O_2$	568.9	0.47	Cancer preventative	[50]
08	30.03	4a-Phorbol 12,13-didecanoate	Phorbol ester	$C_{40}H_{64}O_8$	672.9	0.32	Involves in direct activation of TRPV4	[6]
09	34.21	Octadecane, 1,1'-[1,3-propanediylbis(oxy)] bis	Lipid	$C_{39}H_{80}O_2$	581.1	1.10	Nucleic acid transfer carrier, compound for manufacturing nucleic acid	[41]
10	35.43	25-Norisopropyl-9,19-cyclolanostan-22- en-24-one,3-acetoxy-24-phenyl-4,4,14- trimethyl	Terpenoids	$C_{35}H_{48}O_3$	516.8	5.54	Antibacterial and antifungal activity	[2]
11	36.31	7,8,12-Tri-O-acetyl-3-desoxy-ingol-3-one	-	$C_{26}H_{34}O_9$	490.5	0.54	Antibacterial activity and antioxidant activity	[26]

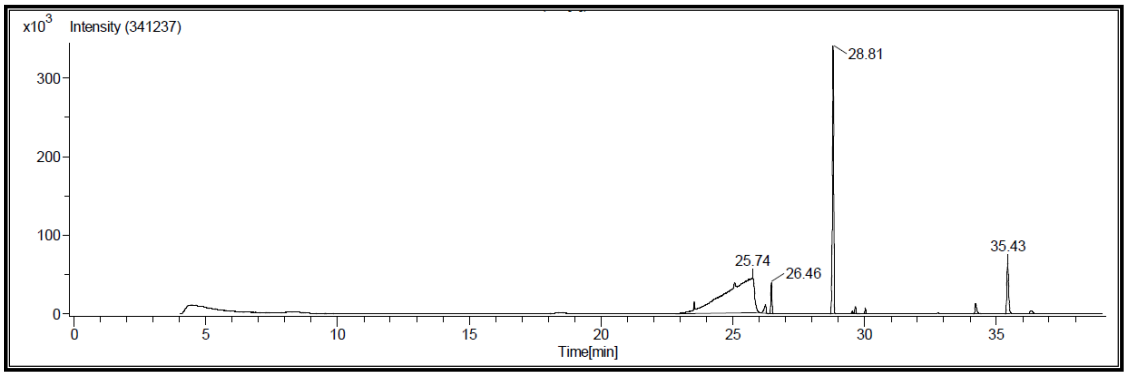

Fig 03: GC-MS chromatogram of the ethanol extract of *Tephrosia purpurea*

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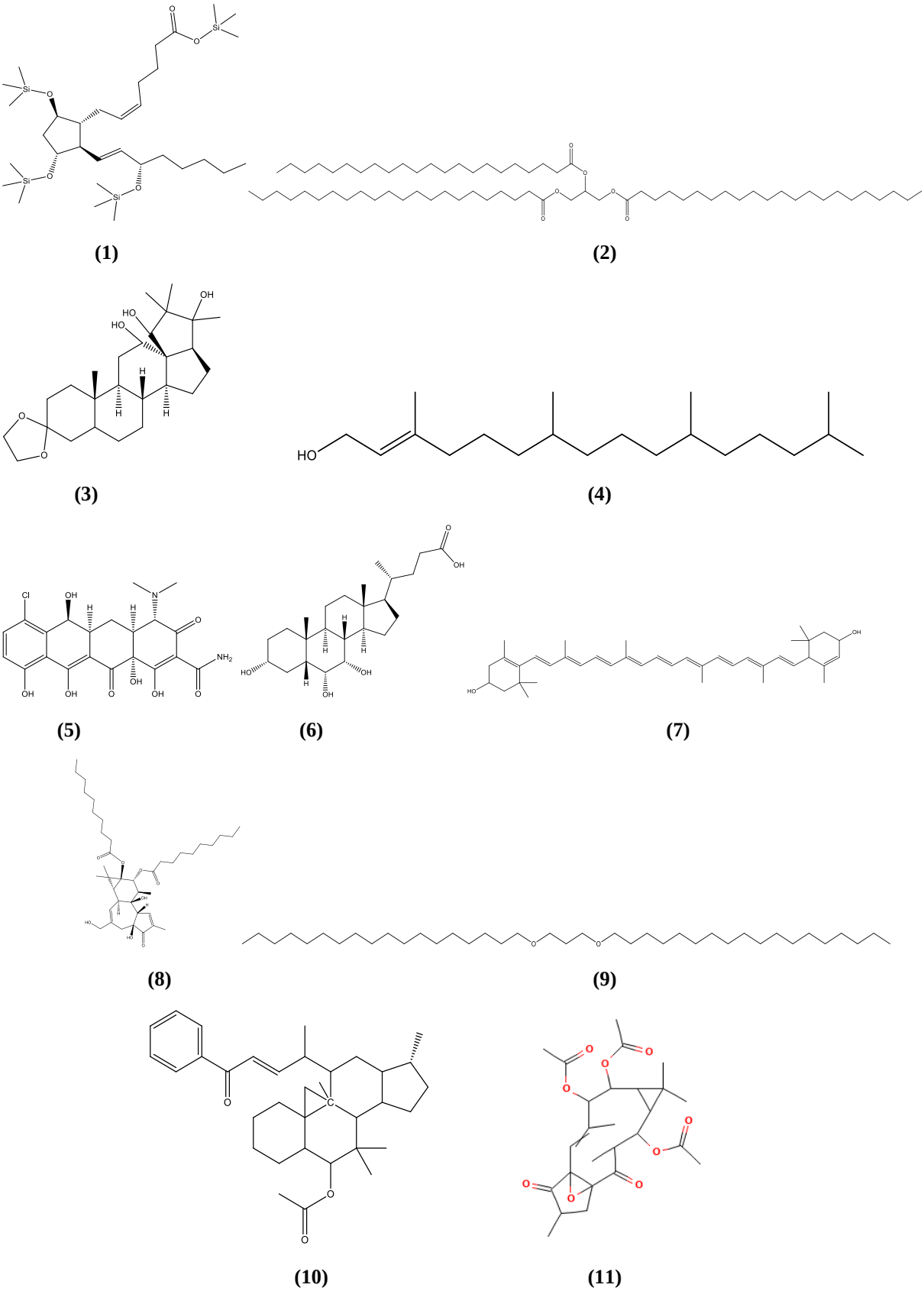

(1) **(2)**

(3) **(4)**

(5) **(6)** **(7)**

(8) **(9)**

(10) **(11)**

Fig. 04: Structure of compound from GC-MS analysis of ethanol extract of *Tephrosia purpurea*

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Table 3: Anti-inflammatory activity of reported phytochemicals (GC-MS analysis) determined by molecular docking (kcal/mol).

Sl. No	Name of the compound	Cox-2 (3mdl)	5LOX (6ncf)	PDE4 (4wcu)	HP5 (1hd2)
1	Indomethacin	-6.7	-7.1	-9.6	-6.5
2	Docosahexaenoic acid, 1,2,3-propanetriyl ester	-7.5	-5.1	-3.7	-3.7
3	10,13-Eicosadienoic acid, methyl ester	-7.5	-6.9	-7.2	-5.5
4	Docosanoic acid nonyl ester	-6.9	-7.3	-6.3	-4.4
5	2-Tridecanone	-5.7	-4.9	-5.5	-4.0
6	Pentacosanoic acid, methyl ester	-6.5	-6.9	-6.3	-4.3
7	n-Hexadecanoic acid	-4.5	-5.4	-5.4	-4.3
8	Phytol	-5.0	-5.9	-6.2	-4.9
9	9,12,15-Octadecatrienoic acid, (Z, Z, Z)-	-6.0	-5.2	-6.4	-5.5
10	2-Benzoylamino-3-(p-tolyl-)-N, N-dimethyl-propenamide	-7.0	-7.5	-8.0	-5.7
11	psi.,. psi. -Carotene, 7, 7', 8, 8', 11, 11', 12, 12', 15, 15'-decahydro	-5.8	-6.8	-8.3	-5.8
12	Pregnane-12,18,20-triol, 18,20-isopropylidene-3,3-ethylenedioxy	-16.2	-13.5	-16.3	-12.1
13	Demeclocycline	-8.0	-8.2	-7.2	-6.7
14	Hyocholic acid	-7.6	-7.5	-8.0	-7.1
15	Xanthophyll	-9.0	-8.3	-8.8	-7.5
16	4a-Phorbol 12,13-didecanoate	-7.4	-7.2	-9.4	-6.1
17	Octadecane, 1,1'-[1,3-propanediylbis(oxy)] bis	-6.1	-4.4	-6.1	-3.6
18	25-Norisopropyl-9,19-cyclolanostan-22- en-24-one,3-acetoxy-24-phenyl-4,4,14- trimethyl	-14.1	-11.8	-14.9	-10.4
19	7,8,12-Tri-O-acetyl-3-desoxy-ingol-3-one	-11.6	-9.7	-12.5	-8.6

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Table 4: Hydrogen bond for bioactive compounds of TP

Sl. No	Name of the compound	Cox-2 (3mdl)		5LOX (6ncf)		PDE4 (4wcu)		HP5 (1hd2)	
		Hydrogen bonds	Distance (Å)	Hydrogen bonds	Distance (Å)	Hydrogen bonds	Distance (Å)	Hydrogen bonds	Distance (Å)
1	Indomethacin	HIS351, LYS358, ASP347, GLN350	1.77292, 2.1851, 2.71613, 3.99205	GLU16, ASP170	2.13907, 3.72686	SER368	3.28683	GLU91, GLY92, LYS93, GLY82	2.33977, 1.92412, 2.77901, 2.22082
2	2-Tridecanone	-	-	ARG138	3.21217	-	-	-	-
3	n-Hexadecanoic acid	-	-	ARG370	1.98162	ASP318, HIS164	2.48526, 3.54875	ASN21, ASN21, GLY17	2.40085, 2.88528, 3.79395
4	Phytol	-	-	-	-	THR333, ASN321	3.25451, 3.58011	-	-
5	9,12,15-Octadecatrienoic acid, (Z, Z, Z)-	HIS207, THR206	2.99813, 2.63123	ARG246	2.51967	-	-	LYS63, LYS63, LYS63, VAL70, LYS93	2.33593, 2.24278, 2.24278, 2.19502, 2.19159
6	2-Benzoylamino-3-(p-tolyl-)-N, N-dimethyl-propenamide	SER471, SER471	3.52274, 3.54603	ARG246, ASP285	2.27844, 3.4514	ASP318	3.69192	GLU16, GLU16	2.6443, 3.47632
7	Demeclocycline	HIS34, HIS133	2.22815, 3.50104	ARG401, GLN15, GLU622	2.55825, 2.68874, 2.55752	THR178, VAL174, ASP391, ASP391, ASN100	2.49339, 2.39228, 2.25327, 2.43289, 3.34449	ASP77, ARG124, ARG124, ARG124, PRO100, ILE119, ILE119	2.26896, 3.35565, 2.93055, 2.89081, 2.34588, 2.83606, 2.87033
8	Hyocholic acid	THR62, LYS468	2.56707, 2.38877	SER171	2.26526	HIS204, SER208, ASP318	2.0572, 1.91824, 1.78516	LYS63, VAL70, GLU16, VAL70, ARG86, VAL69	3.0228, 2.93723, 2.27491, 2.25509, 2.94232, 3.5198

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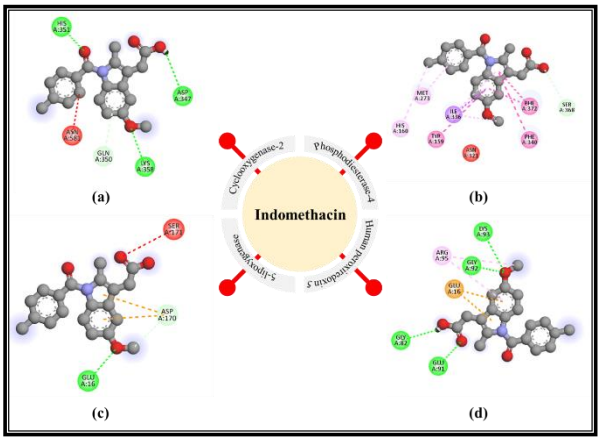

Fig. 5: Molecular docking structure of Indomethacin with (a) Cox-2, (b) PDE4, (c) 5LOX, (d) HP5

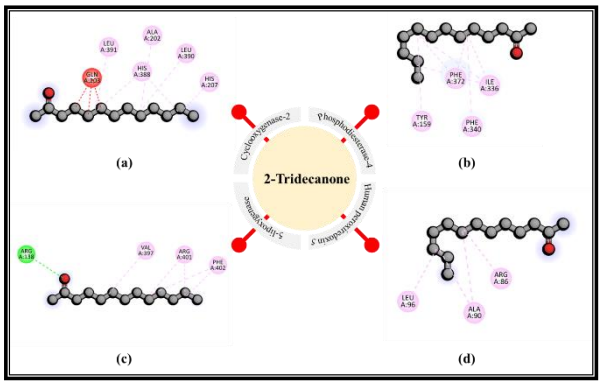

Fig. 6: Molecular docking structure of 2-Tridecanone with (a) Cox-2, (b) PDE4, (c) 5LOX, (d) HP5

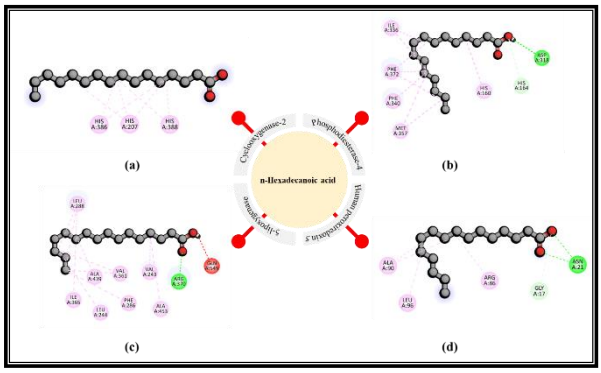

Fig. 7: Molecular docking structure of n-Hexadecanoic acid with (a) Cox-2, (b) PDE4, (c) 5LOX, (d) HP5

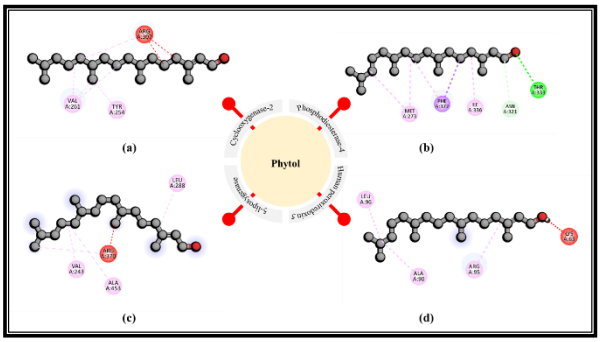

Fig. 8: Molecular docking structure of Phytol with (a) Cox-2, (b) PDE4, (c) 5LOX, (d) HP5

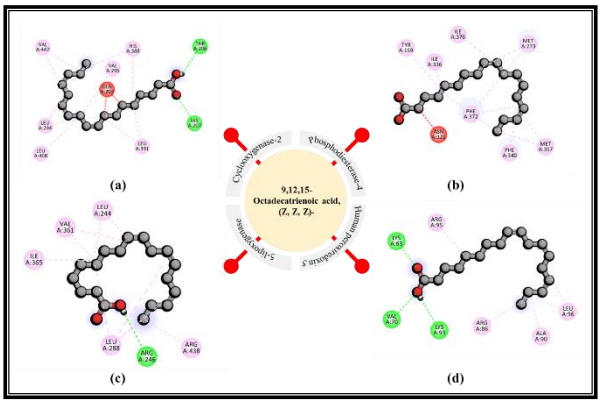

Fig. 9: Molecular docking structure of 9,12,15-Octadecatrienoic acid, (Z, Z, Z)- with (a) Cox-2, (b) PDE4, (c) 5LOX, (d) HP5

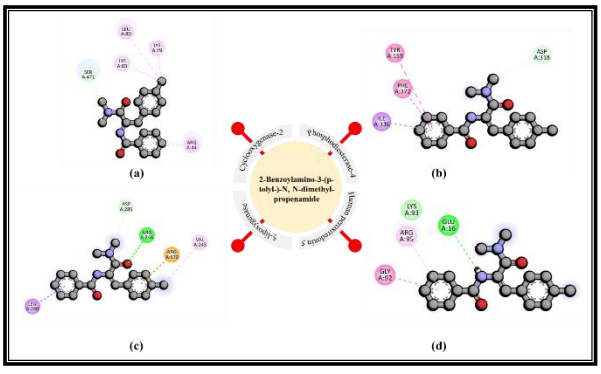

Fig. 10: Molecular docking structure of 2-Benzoylamino-3-(p-tolyl-)-N, N-dimethyl-propenamide with (a) Cox-2, (b) PDE4, (c) 5LOX, (d) HP5

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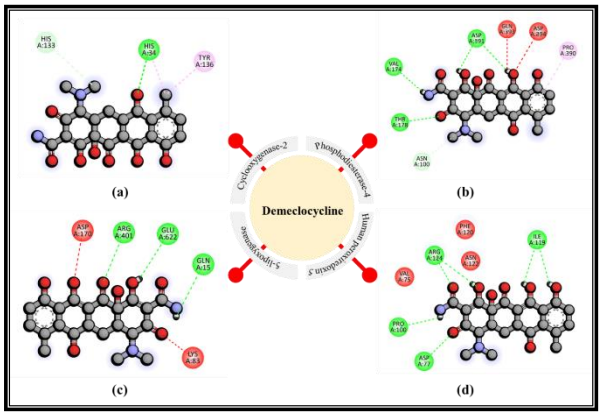

Fig. 11: Molecular docking structure of Demeclocycline with (a) Cox-2, (b) PDE4, (c) 5LOX, (d) HP5

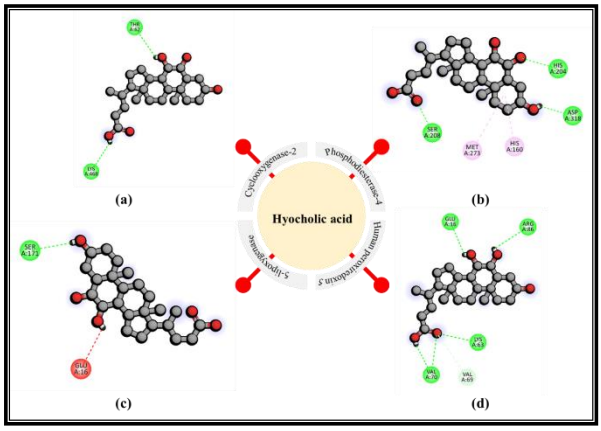

Fig. 12: Molecular docking structure of Hyocholic acid with (a) Cox-2, (b) PDE4, (c) 5LOX, (d) HP5

4. Conclusion

The objective of the current investigation was to identify a variety of bioactive compounds from Tephrosia purpurea in GC–MS analysis. The bioactive compounds are responsible for a variety of pharmacological and therapeutic properties. The investigation also proved the antibacterial, antioxidant, and anti-inflammatory properties of Tephrosia purpurea extracts. It has been confirmed that the plant TP has potential anti-inflammatory activity, as the compounds Pregnane-12,18,20-triol, 18,20-isopropylidene-3,3-ethylenedioxy; 25-Norisopropyl-9,19-cyclolanostan-22-en-24-one,3-acetoxy-24-phenyl-4,4,14-trimethyl; and 7,8,12-Tri-O-acetyl-3-desoxy-ingol-3-one have scored higher than the standard drugs. Our findings suggest that the plant has the potential to support the development of safe and effective medications for a variety of diseases. Additional research is required to evaluate its biological activity and conduct clinical studies to identify novel formulations for medications.

Abbreviation

5LOX: 5-lipoxygenase, ARG: Arginine, ASN: Asparagine, ASP: Aspartic Acid, Cox-2: Cyclooxygenase-2, GC-MS: Gas chromatography-mass spectrometry, GLN: Glutamine, GLU: Glutamic acid, GLY: Glycine, HIS: Histidine, HP5: Human peroxiredoxin 5, ILE: Isoleucine, LYS: Lysine, PDE4: Phosphodiesterase-4, PRO: Proline, SER: Serine, THR: Threonine, TPE: Tephrosia purpurea ethanol extract, TPP: Tephrosia purpurea petroleum ether extract, VAL: Valine.

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Consent for publication

Not applicable

Conflict of interest

The author declares that they have no conflict of interest.

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