Bioactive Compound Profiling and GC-MS Analysis of Ethanol Fraction of *Pavonia zeylonica*

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Abstract

Pavonia zeylonica is one of the medicinally important plants belonging to the family Malvaceae. The present study deals with the GC-MS analysis of the ethanol extract of the above-mentioned plant. The ethanolic leaf extract of P. zeylonica was prepared by standard procedure and concentrated at 40 °C using a hot air oven. We subjected the concentrated ethanol extracts to phytochemical analysis via GC-MS. The GC-MS analyses showed the presence of 37 phytocompounds in the ethanolic extract of the leaf of P. zeylonica, including n-hexadecanoic acid (95.7%), methyl salicylate (97.9%), phytol (96.8%), tetradecane (97.2%), vitamin E (95.6%) and phthalic acid, di(2-propyipentyl) ester (97.7%).

The result of the GC-MS analysis showed that the ethanolic leaf extract of P. zeylonica contains many pharmacologically important bioactive compounds. However, P. zeylonica is an important medicinal plant used in the traditional system of medicine to cure many diseases. So, there is a need for further studies to isolate and identify the specific phytocompounds involved in controlling diseases which may lead to drug development.

Keywords: GC-MS analysis, Bioactive compounds, Pharmaceutical use.

Introduction

India is endowed with an extensive variety of medicinal plants, which have long served as a vital source of natural products for human health. Plants are the most abundant source of medications in ancient systems of medicine, modern medicines, nutraceuticals, food supplements, folk remedies, pharmaceutical intermediates and chemical entities for synthesized compounds. Medicinal plants are a valuable source of medicinal solutions for a variety of diseases. The first scientific studies on the antibacterial effects of plant components were conducted in the final years of the nineteenth century. Plants and plant products have been used for medicinal purposes since the dawn of human civilization.

Over the course of the last century, phytocompounds in plants have played a major role in pharmaceutical production. Phytochemicals are natural bioactive molecules found in various portions of plants, including the root, stem, bark, leaves, seed and fruit. Many traditionally applied plants yield economic advantages.

Pavonia zeylonica belongs to the family Malvaceae and a large shrub of *P. zeylonica* leaves may have both central and peripheral analgesic action and may also possess anti-inflammatory activity by acting through inhibition of prostaglandin biosynthesis. The mature fresh leaves of P. zeylonica have oral anti-inflammatory, analgesic and anti-analgesic properties[16]. Oxygen-derived free radicals and their products are known to play an important role in the pathogenesis of chronic inflammatory disorders. *P. zeylonica* contains many polyphenolic compounds, terpenoids, flavonoids and alkaloids. Polyphenolic compounds have high antioxidant potential, the antioxidant potency of *P. zeylonica* was investigated by employing various established *in vitro* systems. The phytochemical investigation of ethanol extract of *P. zeylonica* leaves revealed the presence of phenolic compounds, tannins, flavonoids, saponins, glycosides. The objective of present study is to identify the phytochemical constituents in ethanol extract of *Pavonia zeylonica* leaves using GC-MS analysis.

Gas chromatography-mass spectroscopy (GC-MS) is a combined analytical technique that detects and identifies chemicals in plant samples. GC MS serves as essential for phytochemical analysis and chemotaxonomic research of medicinal plants containing biologically active components.

Material and Methods

Collection of plant material: The fresh leaves of *Pavonia zeylonica* were collected from the of Thirumalayam Palayam of the Coimbatore city and authenticated by *Pavonia zeylonica* (Ref no: BSI/SRC/5/23/2023-24/Tech- 96) by Dr. M.U. Sharief, Scientist 'F' and Head of Office, Government of India, Ministry of Environment, Forest and Climatic Change, Botanical Survey of India, Southern regional centre, T.N.A.U Campus, Tamil Nadu, India.

Preparation of plant extract: The fresh leaves were washed under running tap water, dried in oven at temperature 40°C and coarsely powdered in a grinder. The powder was extracted with absolute ethanol in Soxhlet extractor at temperature 40-50°C. The extract was dried on water bath at 60°C. GC-MS analysis of this dried ethanol extract was further carried out.

GC-MS Analysis: Gas chromatography-mass spectrometry (GC-MS) is an analytical technique used to identify distinct chemical components in a sample. It provides an overview of the plant extract in terms of its chemical components. The

present study was carried out at the Textile Chemistry Division (TCD), The South India Textile Research Association (SITRA), Coimbatore. The GC-MS analysis used a 7890A gas chromatograph system (Agilent 19091-433HP, USA) and mass spectrophotometer with an HP-5 MS fused silica column (5% phenyl methyl siloxane 30.0 m × 250 µm, film thickness 0.25 µm), interfaced with a 5675C Inert MSD and Triple-Axis detector. Helium gas was employed as a carrier gas and the column velocity flow was set to 1.0 mL/min. Other GC-MS conditions include an ion-source temperature of 250 °C, an interface temperature of 300 °C, a pressure of 16.2 psi, an out time of 1.8 mm and a 1µl injector in split mode with a split ratio of 1:50 at 300 °C.

The column temperature began at 36 °C for 5 minutes and increased to 150 volts at a rate of 4 °C/min. The temperature was raised to 250°C at a rate of 20°C per minute and maintained for 5 minutes. The total elution time was 47.5 minutes. Each component's relative percentage amount was determined by comparing its average peak area to total areas. MS solution software provided by the supplier was used to control the system and capture data[9].

Identification of compounds: The components have been identified using their retention indices and the mass spectrum was analyzed using the National Institute of Standards and Technology's (NIST) database. The database includes more than 62,000 patterns of known chemical compounds. The spectra of the *Pavonia zeylonica* fraction's unknown components were compared to standard mass spectra of known components reported in the NIST library (NISTII)[9].

Results

GC-MS is one of the most effective techniques for identifying volatile matter constituents such as long and branched chain hydrocarbons, alcoholic acids, esters and so on. The result pertaining to GC-MS analysis leads to the identification of the number of compounds from the GC fractions of the ethanolic extract of leaf of *Pavonia zeylonica*. These substances were identified utilizing mass spectrometry combined to GC. The GC-MS chromatogram of the ethanolic leaf extract of *P. zeylonica* showed 37 peaks indicating the presence of 37 compounds. The various components present in the leaf of *P. zeylonica* were detected by the GC-MS shown in figure 1.

The active principles with their peak, retention time (RT), area (%), molecular formula and molecular weight are presented in the table 1. The GC-MS identified compounds show various pharmacological activities as in the table 2.

Discussion

The phytoconstituents are the major important compounds which are responsible for the medicinal properties of the shrubs. Hence medicinal plants could be a potential source for nutraceuticals. The phytochemical substances namely phenols and flavonoids are the major important substances responsible for the medicinal value of the plants including antioxidant, antibacterial, anticancer, anti-inflammatory and anti-diabetic etc. The identification of the phytocompounds was carried out based on the retention time and molecular formula. The names of identified compounds in the *P. zeylonica* with their retention time (RT), molecular formula (MF), molecular weight (MW) and peak area percentage are represented in table 1.

The compounds such as Propane, 2-fluoro-; Silanol, trimethyl-; (S)-4-Ethyl-2-oxazolidone; Benzyl chloride; 2-Pyrrolidinone, 1-methyl-; Phenol, 2-methoxy-; Cyclopentasiloxane, decamethyl-; Methyl salicylate; 3-(4-Methylbenzoyl)-2-thioxo-4-thiazolyl 4-methylbenzoate; Benzoic acid, 2-hydroxy-, ethyl ester; Phenol, 5-ethenyl-2-methoxy-; 2,3-Dimethoxyphenol; Tetradecane; Ethanone, 1-(2,3-dihydro-1,1-dimethyl-1H-inden-4-yl)-; 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-; Diethyl Phthalate; Megastigmatrienone; 1,6,6-Trimethyl-7-(3-oxobut-1-enyl)-3,8 dioxatricyclo [5.1.0.0(2,4)] octan-5-one; 6-Hydroxy-4,4,7a-trimethyl-5,6,7,7a-tetrahydrobenzofuran-2(4H)-one; Neophytadiene; Lidocaine; n-Hexadecanoic acid; Hexadecanoic acid, ethyl ester; 9-Octadecen-1-ol, (Z)-; Phytol; 9,12,15-Octadecatrienoic acid, (Z,Z,Z)-; Dimethylaminoethyl palmitate; Tetracosane; Pentacosane; Phthalic acid, di(2-propylpentyl) ester; Hexacosane; Hentriacontane; Squalene; Sulfurous acid, dodecyl 2-ethylhexyl ester; Hentriacontane; and Vitamin E were present in ethanolic leaf extract of *P. zeylonica*.

Among the identified bioactive components, methyl salicylate (97.9%) has the highest percent peak area. This compound has pain relief, antiseptic, rheumatoid arthritis, skin conditions, topical analgesic cream and anti-inflammatory properties. Phthalic acid, di (2-propylpentyl) ester (97.7%), has to treat several diseases such as malaria, typhoid fever and even snake bite properties. Tetradecane (97.2%): pharmaceutical excipient: ointment, creams and lotions; wound healing; antimicrobial properties; cosmetic applications: lip balms, lipsticks; and moisturizing and emollient properties. Phytol (96.8%) was reported with anti-oxidant, anti-inflammatory, anti-microbial, anticancer, neuroprotective, cardiovascular health, wound healing, skin conditions, respiratory issues and gastrointestinal health activities[2]. n-hexadecanoic acid (95.7%) was reported as having antioxidant, hypocholesterolemic, nematicide, pesticide, lubricant, antiandrogenic, hemolytic, 5-alpha reductase inhibitor and antipsychotic properties[2].

Conclusion

In the present study, the identified phytocompounds in the ethanol leaf extract of *P. zeylonica* may be used for drug development. This study may also enhance the traditional usage of *P. zeylonica* due to its bioactive compounds identified by GC-MS analysis.

Table 1
GC-MS analysis revealed the presence of phytochemical component in ethanol leaf extract of *Pavonia zeylonica*

S.N.	Component RT	Compounds Name	Molecular Formula	Molecular weight (g/mol)	Area %
1.	3.6276	Propane, 2-fluoro-	C_3H_7F	62.09	63.4
2.	4.8352	Silanol, trimethyl-	$C_3H_{10}OSi$	90.02	71.0
3.	6.2597	(S)-4-Ethyl-2-oxazolidone	$C_5H_9NO_2$	115.13	74.8
4.	8.0487	Benzyl chloride	C_7H_7Cl	126.58	94.7
5.	8.8705	2-Pyrrolidinone, 1-methyl-	C_5H_9NO	99.13	85.3
6.	9.8604	Phenol, 2-methoxy-	$C_7H_8O_2$	124.14	83.4
7.	11.3910	Cyclopentasiloxane, decamethyl-	$C_{10}H_{30}O_5Si_5$	370.77	82.9
8.	12.4123	Methyl salicylate	$C_8H_8O_3$	152.15	97.9
9.	13.4776	3-(4-Methylbenzoyl)-2-thioxo-4-thiazolyl 4-methylbenzoate	$C_{19}H_{15}NO_3S_2$	369.5	81.1
10.	14.4256	Benzoic acid, 2-hydroxy-, ethyl ester	$C_9H_{10}O_3$	166.17	93.0
11.	15.7876	Phenol, 5-ethenyl-2-methoxy-	$C_9H_{10}O_2$	150.17	86.5
12.	16.9761	2,3-Dimethoxyphenol	$C_8H_{10}O_3$	154.16	74.6
13.	17.8435	Tetradecane	$C_{14}H_{30}$	198.39	97.2
14.	18.8367	Ethanone, 1-(2,3-dihydro-1,1-dimethyl-1H-inden-4- yl)-	$C_{13}H_{16}O$	188.26	82.1
15.	19.5336	4-(2,6,6-Trimethylcyclohexa-1,3-dienyl) but-3-en-2- one	$C_{13}H_{18}O$	190.28	90.7
16.	20.3370	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	$C_{11}H_{16}O_2$	180.24	82.2
17.	21.3425	Diethyl Phthalate	$C_{12}H_{14}O_4$	222.24	94.2
18.	21.7442	Megastigmatrienone	$C_{13}H_{18}O$	190.28	89.3
19.	22.5418	1,6,6-Trimethyl-7-(3-oxobut-1-enyl)-3,8-dioxatricyclo[5.1.0.0(2,4)]octan-5-one	$C_{13}H_{16}O_4$	236.26	74.7
20.	23.5600	6-Hydroxy-4,4,7a-trimethyl-5,6,7,7a-tetrahydrobenzofuran-2(4H)-one	$C_{11}H_{16}O_3$	196.24	94.1
21.	24.2041	Neophytadiene	$C_{20}H_{38}$	278.5	94.1
22.	24.9867	Lidocaine	$C_{14}H_{22}N_2O$	234.34	93.3
23.	25.5944	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	256.42	95.7
24.	25.9003	Hexadecanoic acid, ethyl ester	$C_{18}H_{36}O_2$	284.5	90.2
25.	26.6884	9-Octadecen-1-ol, (Z)-	$C_{18}H_{36}O$	268.5	94.0
26.	27.3107	Phytol	$C_{20}H_{40}O$	296.5	96.8
27.	27.6394	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	$C_{18}H_{30}O_2$	278.4	87.6
28.	29.0765	Dimethylaminoethyl palmitate	$C_{20}H_{41}NO_2$	327.5	80.8
29.	30.1284	Tetracosane	$C_{24}H_{50}$	338.7	81.7
30.	31.0006	Pentacosane	$C_{25}H_{52}$	352.7	89.6
31.	31.4713	Phthalic acid, di(2-propylpentyl) ester	$C_{24}H_{38}O_4$	390.6	97.7
32.	31.8230	Hexacosane	$C_{26}H_{54}$	366.7	88.4
33.	32.6038	Hentriacontane	$C_{31}H_{64}$	436.8	90.4
34.	33.6491	Squalene	$C_{30}H_{50}$	410.7	93.4
35.	35.1725	Sulfurous acid, dodecyl 2-ethylhexyl ester	$C_{20}H_{42}O_3S$	362.6	61.4
36.	36.3509	Hentriacontane	$C_{31}H_{64}$	436.8	79.5
37.	36.9703	Vitamin E	$C_{29}H_{50}O_2$	430.7	95.6

Table 2
GC-MS analysis revealing the presence of phytochemical component in ethanol leaf extract of *P. zeylonica* and their biological activities

S.N.	Compounds Name	Nature of Compounds	Bio-Activity
1.	Propane, 2-fluoro-	Organic compound	-
2.	Silanol, trimethyl-	Organosilicon	Antimicrobial Properties
3.	(S)-4-Ethyl-2-oxazolidone	Miscellaneous	Antibacterial, Anti- viral
4.	Benzyl chloride	Aromatic compound	Perfumes, flavors and pharmaceuticals (Antibiotics, Anti-inflammatory, Anesthetics)
5.	2-Pyrrolidinone, 1-methyl-	Polar organic solvent	Anesthetic formulation, Antimicrobial and Wound healing
6.	Phenol, 2-methoxy-	Unsaturated Aromatic compound	Antioxidant, Antiseptic, Anti- inflammatory and Antimicrobial
7.	Cyclopentasiloxane, decamethyl-	Organosilicon compound	Wound healing, Drug delivery system, Skincare products
8.	Methyl salicylate	Salicylic acid (Organic liquid)	Pain Relief and Anti-inflammatory, Antiseptic, Rheumatoid arthritis, Analgesic for joint pain
9.	3-(4-Methylbenzoyl)-2-thioxo-4-thiazolyl 4-methylbenzoate	Organic compound	Anti- inflammatory, Antimicrobial, Antioxidant, Cytotoxic (anti-cancer) and Neuroprotection[12]
10.	Benzoic acid, 2-hydroxy-, ethyl ester	Organic compound (o-hydroxybenzoic acid esters	Pain Management: Headaches, muscle aches, arthritis, Wound healing, Anti-inflammation, Antimicrobial
11.	Phenol, 5-ethenyl-2-methoxy-	(Methoxyphenol) Volatile compound	*In vitro* and *In vivo* Anti-cancer activity[2]
12.	2,3-Dimethoxyphenol	Phenylpropanoid	Anti-Pyretic, Analgesic and Antiseptic
13.	Tetradecane	Alkanes Hydrocarbon	Cosmetic and Pharmaceutical Preparations (Creams, ointments, Capsules and Tablets)
14.	Ethanone, 1-(2,3-dihydro-1,1-dimethyl-1H-inden-4- yl)-	Tetralin compound	-
15.	4-(2,6,6-Trimethylcyclohexa-1,3-dienyl) but-3-en-2- one	Sesquiter Penoid Compound	Pain Management, Skin conditions, Infections and Neurodegenerative diseases
16.	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	Phenolic, Lipophilic compound	Antioxidant, Antimicrobial, Anti-cancer properties and Cardiovascular protection
17.	Diethyl Phthalate	Organic acid	Antimicrobial plasticizer in a wide variety of consumer goods[6].
18.	Megastigmatrienone	C13 nor-isoprenoid derived from carotenoids (terpene)	Aroma Nature, Cytotoxic Activity[2,3]
19.	1,6,6-Trimethyl-7-(3-oxobut-1-enyl)-3,8 dioxatricyclo [5.1.0.0(2,4)] octan-5-one	Phthalic acid mono ester	Hypertension, Heart failure, Asthma, Chronic obstructive pulmonary diseases, Obesity, Glaucoma treatment
20.	6-Hydroxy-4,4,7a-trimethyl-5,6,7,7a-tetrahydrobenzofuran-2(4H)-one	Hydroxyl Chemical compound	-
21.	Neophytadiene	Terpenoid	Antimicrobial[3].
22.	Lidocaine	Monocarboxylic acid amide & tertiary amino compound	Anti-arrhythmic, Antimicrobial, Pain relief, Burns, Neuropathic pain and Cancer pain, All Pain Management
23.	n-Hexadecanoic acid	Palmitic acid (Saturated fatty acid)	Antioxidant, Hypocholesterolemic, Nematicide, Pesticide, Lubricant, Antiandrogenic, Hemolytic, 5-alpha reductase inhibitor, antipsychotic[2,5]
24.	Hexadecanoic acid, ethyl ester	Palmitic acid ester	Antioxidant, Hypocholesterolemic nematicide, pesticide, anti-androgenic flavor, hemolytic, 5-Alpha reductase inhibitor[4,7,10].

25.	9-Octadecen-1-ol, (Z)-	Unsaturated alcoholic compounds	No activity reported[2].
26.	Phytol	Diterpene	Antimicrobial, Anti-inflammatory, Anticancer, Diuretic, Antifungal against *S. typhi*, Neuro protective, cardio vascular health, wound healing and Gastro intestinal health[1,10].
27.	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	Liolenic acid	Anti-inflammatory, Hypocholesterolemic cancer preventive, hepatoprotective, nematicide, anti-histaminic anti-eczemic, anti-acne, 5-Alpha reductase inhibitor, anti-androgenic, anti-arthritic, anti-coronary[4,8,10].
28.	Dimethylaminoethyl palmitate	Palmitic acid	Antimicrobial, Anti-inflammatory Properties
29.	Tetracosane	Higher alkane	Antioxidant / Anti corrosive, Anti-inflammatory, Antibacterial, used in peptic ulcer treatment[1].
30.	Pentacosane	Higher alkane	Antimicrobial, Anti-inflammatory, Cytotoxic,
31.	Phthalic acid, di(2-propylpentyl) ester	Bicyclic aromatic hydrocarbon ester	To treat several diseases such as malaria, typhoid fever and even snake bites
32.	Hexacosane	Higher alkane	Antioxidant, Antifungal and Anti-inflammatory
33.	Hentriacontane	Higher alkane	Antifungal against fungal spores germination, Antioxidant, Anti-tumor, Antibacterial[2].
34.	Squalene	Triterpene	Antibacterial, Anti-oxidant, Pesticide, Antitumor, Cancer preventive, Immunostimulant, Chemo preventive, Lipoxygenase-inhibitor[5].
35.	Sulfurous acid, dodecyl 2-ethylhexyl ester	Organic compound	Anti-Nociceptive, Anti-Pyretic, Cardiovascular protection Wound healing
36.	Hentriacontane	Higher alkane	Antifungal against fungal spores germination, Antioxidant, Anti-tumor, Antibacterial[2].
37.	Vitamin E	Vitamin E	Anti-ageing, analgesic, anti-diabatic anti-inflammatory, anti-oxidant, anti-dermatitic, anti-leukemic, anti-tumor, anti-cancer, hepatoprotective, Hypocholesterolemic, anti-ulcerogenic, anti-spasmodic, anti-bronchitic, anti-coronary[5].

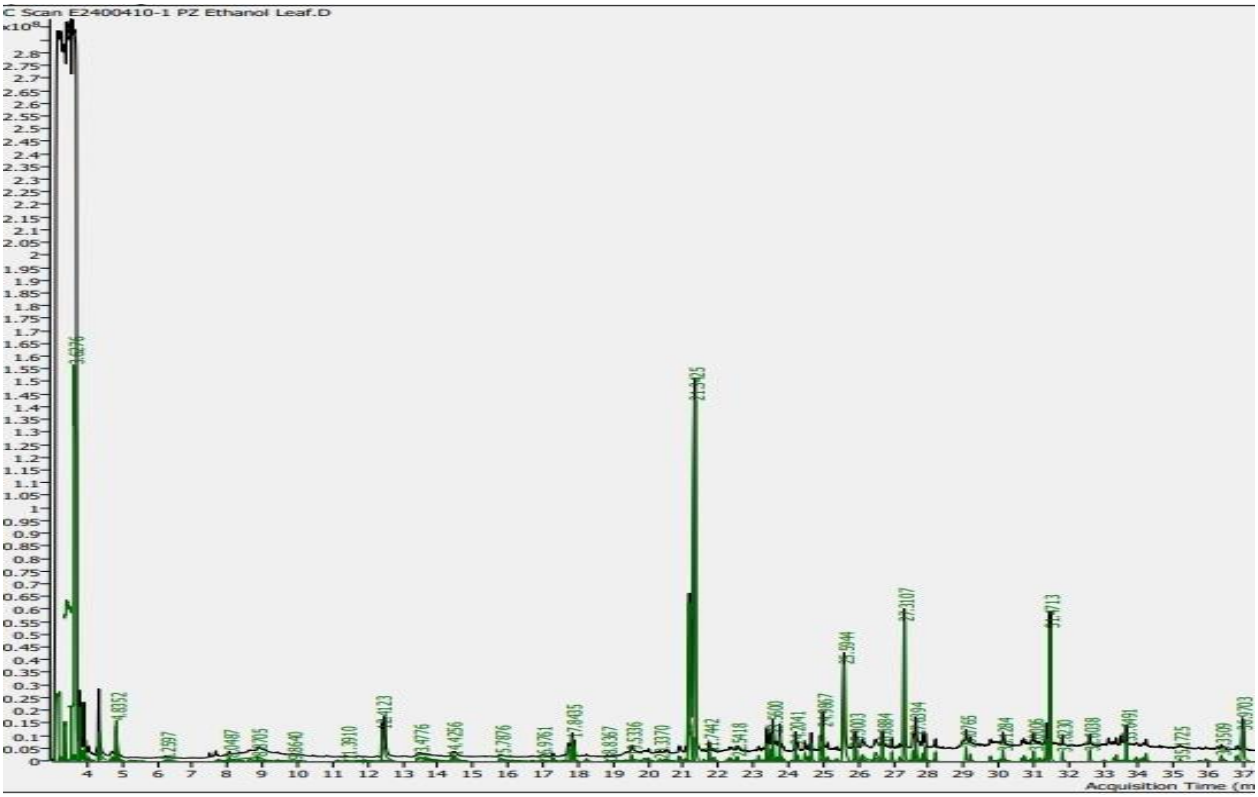

Figure 1: GC-MS Chromatogram of ethanolic extract of leaf of *Pavonia zeylonica*

Further investigation is required for the pharmacological activity of specific compounds of *P. zeylonica*, which may lead to the development of new drugs for the treatment of specific diseases. Thus, GC-MS analysis is the first step towards understanding the nature of active principles in the ethanal leaf extract of *P. zeylonica*.

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(Received 28th October 2024, accepted 03rd January 2025)