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PHYTOCHEMICAL SCREENING OF SCOPARIA DULCIS LINN. SCROPHULARIACEAE AND IN SILICO BIOACTIVITY STUDY OF ISOLATED COMPOUNDS

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ABSTRACT

The plant Scoparia dulcis Linn. belongs to the family Scrophulariaceae, Known as a sweet broom, Scoparia dulcis Linn. is a tropical American natural plant that is a member of the Scrophulariaceae family. Its anti-diabetic, antipyretic, antihypertensive, and diuretic properties were recognized by traditional healers, who have used it to create a number of promising traditional medications and formulations. By using preliminary phytochemical analysis, column chromatography to separate active chemicals, and spectrum analysis such as UV, IR, NMR, and MASS spectra to describe the isolated component, the current study's primary goal is to identify the phytoconstituents contained in the leaf extract. The plant has more phytochemicals, including carbohydrates, alkaloids, tannins, phenols, flavonoids, vitamin C, and amino acids, according to the early phytochemical analysis. According to the quantitative calculation, it contains a significant amount of flavonoids, phenols, and vitamins C. To separate the phytoconstituents, the ethanol extract was made and used in through chromatography. It was found that the percentage of acetone:ethanol (60:40) and (40:60) included a dull white crystalline substance. Spectral analyses were performed on this substance. The spectrum investigations suggest the existence of several functional groups from the elemental analysis. It is possible to identify the separated compound's chemical makeup based on the spectrum analyses. Future research might also focus on identifying novel chemicals and their potential medical uses.

KEYWORDS: anti-diabetic, antipyretic, antihypertensive, traditional medications, phytoconstituents.

1. INTRODUCTION

The intricate blend of compounds that plants naturally produce are known as phytochemicals, and they serve as a crucial foundation for nutritional sciences and phytotherapy. While some have lately been the focus of scientific investigation, others are just partially defined.[1] There are several photochemicals found in plant sources, but their chemical makeup and potential uses are unknown. As the global market for photochemicals for pharmaceuticals, medications, food and health goods, nutraceuticals, and cosmetics continues to develop, methods have been created in order to isolate and characterize phytochemicals.[2] Scoparia dulcis L. is a tiny herb that is used medicinally and is a member of the Scrophulariaceae family. It is Known as "sweet broom," this plant grows as a wasteland in wetland areas and throughout tropical and subtropical regions.[3] It has numerous therapeutic uses and is utilized in ancient medical systems.[4] Numerous potential traditional medicinal applications have been created by traditional healers. It is used to treat hypertension in Taiwan and diabetes.[5] in India.

It has been used to heal wounds and hemorrhoids in Brazil and to treat sickle-cell disease in Nigeria.[6] Due to the presence of the phytoconstituent Scoparinol.[13] this plant has demonstrated good antioxidant.[7] analgesic.[8] anti-inflammatory.[9] anti-ulcer.[10] antiurolithiatic.[11] hyperlipidemic.[12] and antibacterial qualities. Scoparic acid, Scopadulcic acids.[14] Scopadulcinol, and Scopadulin are among the other active ingredients found in this plant.[15] Diterpene.[16] triterpenes.[17] and flavonoids, which are found in the plant's aerial portion, are responsible for the antidiabetic effects of this plant. Given this context, the goal of the current study is to uncover novel phytoconstituents found in plant leaves. The aim of this study is to determine the bioactive compounds present in the Scoparia dulcis L. leaves extract with the aid of UV-VIS, FTIR, NMR, and MASS Spectral Techniques, which may provide an insight in its use of traditional medicine.

2. MATERIALS AND METHODS

2.1 PREPARATION OF EXTRACTS OF Scoparia Dulcis Linn

2.1.1 Procedure of Pet. Ether Extract

In a Soxhlet extractor, 300 g of powdered Scoparia Dulcis Linn were extensively defatted using petroleum ether at 60 to 80 °C. Petroleum ether extracts (PEE) were produced by extracting the solvent under pressure, yielding 5.6 g of a dark greenish brown oily material that was refrigerated. The resultant marc was meticulously extracted repeatedly using solvents of increasing polarity, concentrated under low pressure, and labelled as such. It was then left to air dry at room temperature. The petroleum ether extract of the plant's seeds was picked up in petroleum ether after being saponified with 1M alcoholic KOH to remove any fatty components, and thesolvent was thenevaporated to create 3g of unsaponified material. There are fewer components in this fraction than in the unsaponified extract.[18]

2.1.2 Procedure of Ethanolic Extract

Scoparia Dulcis Linn were collected, finely sliced, and allowed to dry in ambient air. First, 250 g of the dried Withania somnifera Linn. roots were obtained, and using a Soxhlet apparatus and ethanol as the solvent, the seeds were extracted at a temperature of around 78 °C. Second, a rotary evaporator was used to condense this fraction at lower pressure so that a concentrated extract could be produced. The extract was then put through a GCMS analysis to determine what phytochemicals were present. In order to identify the phytochemicals that were dissolved in different solvent polarities, extraction employing other solvents (petroleum ether and ethyl acetate) in the same technique was also carried out.[19]

3. EXTRACTS PHYTOCONSTITUENTS HAVE TO BE IDENTIFIED

The following phytoconstituents were found in *Scoparia dulcis Linn.* during a preliminary phytochemical screening.

Name of Tests	Pet. ether	Ethanolic Extract
CARBOHYDRATES		
Molish Test	+	+
Fehling's test	+	+
Benedict's test	+	+
PROTEIN		
Biuret test	+	-
Millon's test	-	-
Precepitation test	-	-
ALKALOIDS		
Mayer's test	-	+
Hager's test	-	+

Wagner's test	-	+
Dragendorff's test	-	+
GLYCOSIDES		
Keller-kiliani test	+	+
Baljet test	+	+
STEROIDS		
Salkowski test	+	+
FLAVONOIDS		
Lead acetate	+	+
NaOH solution	+	+
TANNINS		
5% $FeCl_3$ solution test	-	+
Dil. Iodine solution	-	+
Dil HNO_3	-	+
SAPONINS		
Foam test	+	+
TERPENOIDS		
Salkowski'stest	+	+
Ethyl acetate and DilNH_3 solution	+	+
Fatty acid and oils	+	+

4. TLC STUDY ON THE EXTRACTS

In chromatographic method, different substances are separated differently between a mobile and a stationary phase. In thin layer chromatography, the stationary phase is a solid adsorbent whereas mobile phase is always a liquid and the technique is widely applicable for identifying components in a sample as well as for preparative purposes.[20]

The crude extracts of Scoparia dulcit L. (SPE, SEA, SAc and SM) were subjected to TLC in solvents of different polarity range at different ratios. Each of the four extracts were run in five different solvent systems viz., PE (100%), PE: EA=9:1, PE: EA=4:1, PE: M=9.5:0.5 and PE: EA: M= 8:1:1 on analytical plates over Silica gel (TLC grade, Merck India). In each case, the coloured components of the sample were observed directly, while the colourless components were visualized by shining ultraviolet light (365 nm), iodine vapour or by spraying the plates with $K_2Cr_2O_7$. Finally, the Rf values of each were calculated out.[21]

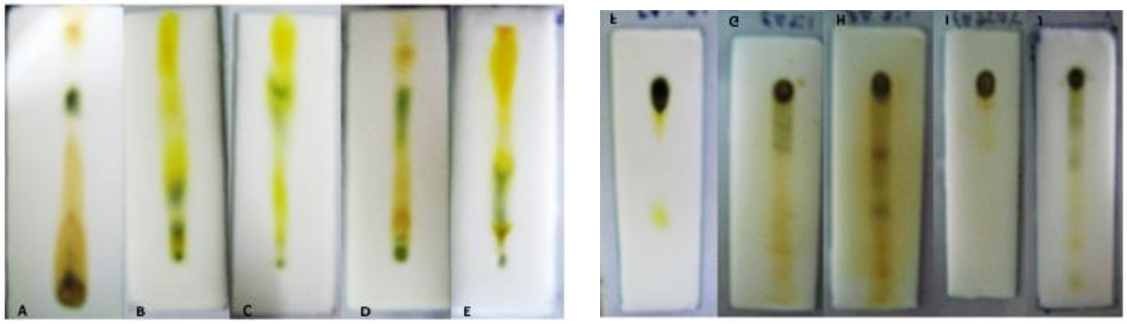

Figure 1- TLC profiling of Petroleum ether extract.

Figure 2- TLC profiling of Petroleum ether extract.

5. Isolation techniques of bioactive compounds by chromatographic

For the isolation of pure secondary metabolite, Silica Gel (mesh size б0-120) was used as a stationary phase and was activated by heating at 120 o C for an hour in Hot Air Oven to remove moisture. The packing of column was done by slurry method. Special caution was taken to avoid any cracks, air bubbles or channels. The sample was prepared by mixing a part of the activated silica gel with concentrated plant extract followed by air drying and loading into the column. Eluent of different solvent ratios was continuously poured into the column and a definite amount of eluted solvent was collected in separate marked conical flasks.[22] Observing the mobility of different components, polarity of the eluent was gradually increased by adding a moderately polar solvent such as ethyl acetate. the eluent moved through the stationary phase, different components present in the sample also started moving downward at different rates depending on their size and molecular weight and thus they got separated. Each of the fractions collected were concentrated using Rotary evaporator, tested purity in TLC and was further separated by preparative TLC and preparative HPLC (High Performance Liquid Chromatography).

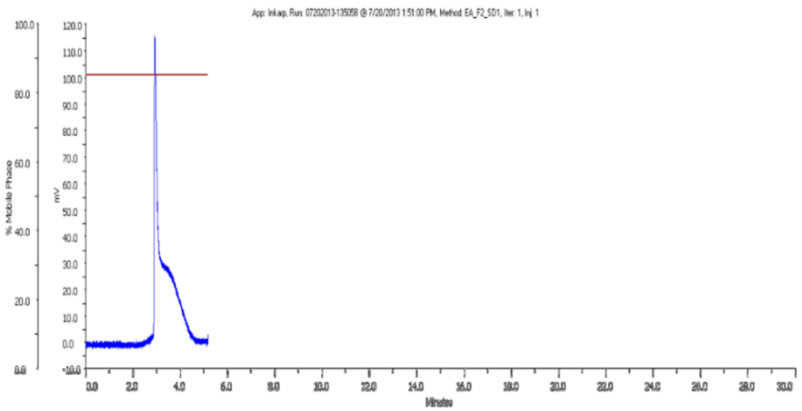

Fig 3: Preparative HPLC Chromatogram of the compound.

6. Structure elucidation of the isolated compound by Spectroscopic data analysis

6.1 Fourier-transform Infrared spectroscopy (FTIR)

Fourier-transform Infrared spectroscopy is one of the most important analytical techniques used to determine the chemical functional groups in a sample. It can be employed to study virtually any sample in virtually any state whether it is liquid, solution, paste, powder, film, fibre, gas or surface with a judicious choice of sampling technique. The most significant development in infrared spectroscopy has come up with the introduction of Fourier-transform spectrometer which provides an intensely enhanced quality of the spectra as well as minimization of time requirement in obtaining data. In addition, with continuous developments of computer, infrared spectroscopy has made further progresses. This is based on the principle of vibrations of the atoms of a molecule. An infrared spectrum is usually obtained by a passage of infrared radiation through a sample, specifying what portion of the incident radiation is absorbed at a particular energy. The energy specifying any peak in an absorption spectrum is related to the frequency of vibration of a portion of the sample molecule. Thus, IR spectroscopy provides a significant and standard tool for structure elucidation and compound identification.[23]

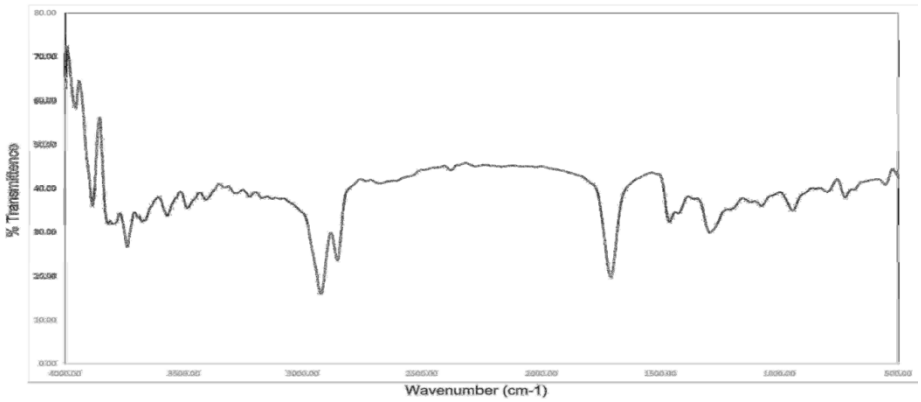

Fig 4: FT-IR spectrum of the compound.

6.2 Nuclear Magnetic Resonance (NMR) spectroscopy

Nuclear Magnetic Resonance spectroscopy has made a remarkable influence in many areas of chemistry, biology, medicine and is widely applicable in determining the structure of the molecules. NMR spectroscopy makes usage of radiofrequency radiation to generate transitions among different nuclear spin states of samples in a magnetic field. The effectiveness of NMR spectroscopy for structural characterization arises as different atoms in a molecule experience slightly different magnetic fields and transitions at somewhat different resonance frequencies in an NMR spectrum. the spectra lines arise due to interactions

between different nuclei Moreover, splitting of that deliver information about the proximity of different atoms in a molecule. NMR provides information about individual hydrogen and carbon atoms in the structure, allowing comprehensive reconstruction of the molecule's architecture. 1H NMR or proton NMR and 13C NMR or carbon NMR are one dimensional NMR used for identification of hydrogen-1 nuclei and carbon atoms respectively within the molecule structure of its molecule. DEPT (Distortionless of a substance in order to determine the Enhancement by Polarization Transfer) allows determining the multiplicity of carbon atom substitution with hydrogen.[24-25]

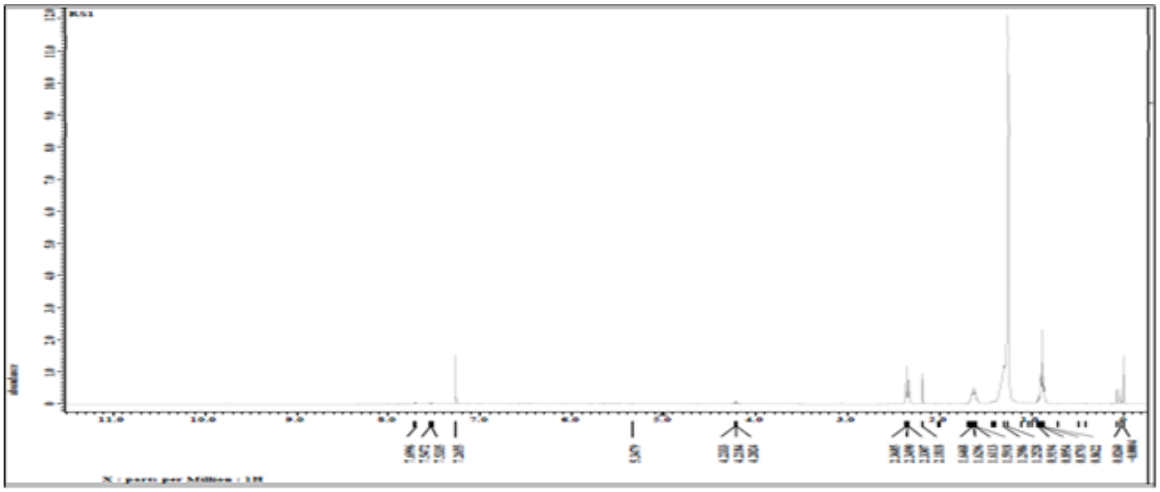

Fig 5: 1H-NMR spectrum of the compound.

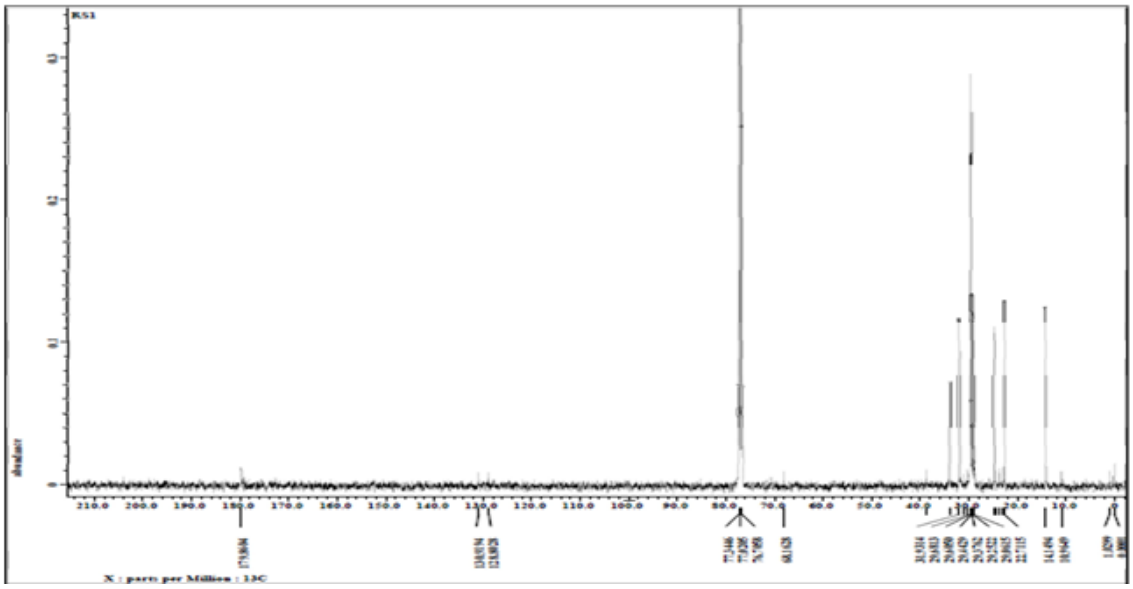

Fig 6: 13 C-NMR spectrum of the compound.

6.3 Mass Spectrometry (MS)

Mass spectrometry is an analytical technique which measures mass-to-charge ratio of charged particles and is widely applicable to determine the mass as well as elemental composition of a sample or molecule. The principle of mass spectrometry is based on the involvement of ionizing chemical compounds that produce charged molecules or moleculefragments followed by measurement of their mass-to-charge ratios by one of a techniques such as EI, CI, ESI, APCI or MALDI. MS consists of three main variety of components; an ion source to generate gaseous ions from the material being studied, resolving ions into their characteristic masses according to their mass-to- an analyzer for charge ratio and a detector for detecting and recording each of the resolved ionic types. Furthermore, a sample introduction system to admit the sample and a computer to control the instrument, acquire and manipulate data as well as to compare spectra to present.[26]

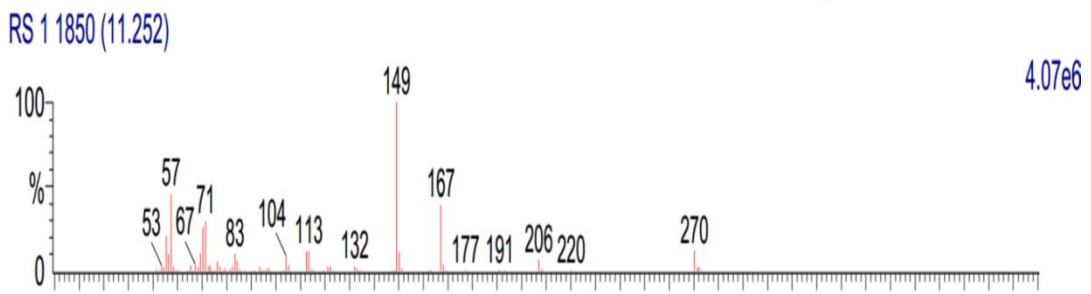

Fig 7: Mass spectrum of the compound.

CONCLUSION

Summary Scoparia dulcit L. is a distinguished folk medicinal plant and amongst the indigenous communities it has been broadly practised for its diverse pharmacological properties. Literature survey reflects that Scoparia dulcit L. possesses a wide range of phytoconstituents belonging to different groups of secondary metabolites. The experimentations on crude extracts as well as isolated metabolites to investigate the potential pharmacological possessions had documented its wide potentialities to exhibit analgesic, anti-inflammatory, antidiabetic, antioxidant, antiviral, antitumor, cytotoxic and hepatoprotective activities evaluated in both in vivo and in vitro. Although many researches have already been carried out in different parts of the world, very little work has been documented from North Eastern region of India, especially from Assam. Again, no work related to computational screening of the compounds from this plant reported yet. Hence, the present state of work was an attempt to investigate the has been phytochemical screening of Scoparia dulcit L.

from Southern Assam as well as in tilico evaluation of the potential bioactivity of the isolated metabolite (s).

Regarding chromatography, isolation of bioactive compound(s), by employing Column a TLC grade pure fraction was isolated from Ethyl acetate extract of Scoparia dulcit L., using Petroleum ether and Ethyl acetate (9:1) as eluent. The fraction was further purified in pHPLC and the pure compound was isolated. After analyses and interpretation of different spectroscopic data generated by Infrared spectroscopy (IR), Nuclear Magnetic Resonance spectroscopy (NMR) and Mass spectrometry (MS), thestructure of the compound was elucidated and found to be (E)-7-methyl-2-(5,6,7,8- tetrahydronaphthalen-2-yl)oct-5-en-3-one, a ketonic compound. the compound has not been reported previously from Scoparia dulcis.

REFERENCES

1. John T, Rachel A, John M and Romeo T: Phtochemistry of medicinal Plants, Springer Science & Business Media, 2013; 1-11.
2. Meskin and Mark S: Phytochemicals in Nutrition and Health. CRC Press 2002; 123.
3. Gamble JS: Flora of the Presidency of Madras. Vol I, II, III. Botanical Survey of India, Calcutta, India, 1935.
4. Bieski GC, Rios F, Santos RM and Oliveira De: Ethnopharmacology of medicinal plants of the Pantanal region (Mato Grosso, Brazil). Evidence-Based Complementary and Alternative Medicine, 2012; II: 36.
5. Pari L and Eswaran SV: Hypoglycemic activity of Scoparia dulcis L. extract in Alloxan induced hyperglycemic rats: Phytotherapy Research, 2002; 16(7): 662-64.
6. Pamunuwa G, Karunaratne N and Waisundara VY: Antidiabetic Properties, Bioactive Constituents, and Other Therapeutic Effects of Scoparia dulcis. Evidance - based Complementary and Alternative Medicine, 2016; ID 8243215: 1- 11.
7. Latha M and Pari L: Effect of an aqueous extract of Scoparia dulcis on blood glucose, plasma insulin and some polyol pathway enzymes in experimental rat diabetes. Brazilian Journal of Medical and Biological Research, 2004; 37(4): 577-86.
8. Zulfiker AHM, Rahman M, Hossain MK, Hamid K, Mazumder MEH and Rana MS: In vivo analgesic activity of ethanolic extracts of two medicinal plants - Scoparia dulcis L. and Ficus racemosa Linn. Biology and Medicine, 2010; 2(2): 42-48.
9. Tsai JN, Peng WH, Chiu TH, Lai SC and Lee CY: Antiinflammatory Effect of Scoparia

dulcis L. and Betulinica Acid. The American journal of Chinese Medicine, 2011; 39: 948-56.

10. Schronerová K, Paul A and Sourivong B: Antiulcer activity of water extract of Scoparia dulcis Melánia Babincová a, Fitoterapia, 2008; 79: 587-88.
11. Ida VE, Christi R and Rai S: A comparative study of antilithiatic effect of three customary plants and their antioxidant activity. World Journal of Pharmaceutical Sciences, 2014; 4(5): 1290 -299.
12. Pari L and M Latha: Antihyperlipidemic effect of Scoparia dulcis (Sweet Broomweed) in streptozotocin diabetic rats. Journal of Medicinal Food, 2006; 9(1): 102-07.
13. Yisa J and Minna: Phytochemical Analysis and antimicrobial activity of Scoparia dulcis and Nymphaea lotus. Australian Journal of basic and Applied Sciences, 2009; 3(4): 3975-979.
14. Hayashi T, Kawasaki M and Okamura K: Scoparic acid A, a β-Glucuronidase inhibitor from Scoparia dulcis. Journal of Natural Products, 1992; 55(12): 1748-755.
15. Hayashi T, Kishi M and Kawasaki M: Scopadulcic acid-A and -B, new diterpenoids with a novel skeleton, from a Paraguayan crude drug ‘typychá kuratũ’ (Scoparia dulcis L.),” Tetrahedron Letters, 1987; 28(32): 3693-696.
16. Mahato SB, Das MC and Sahu NP: Triterpenoids of Scoparia dulcis. Phytochemistry, 1981; 20(1): 171-73.
17. Lisdonk EH, Rutten GE and Weel CV: α-Glucosidase inhibitors for patients with type 2 diabetes. results from a Cochrane systematic review and meta-analysis. Diabetes Care, 2005; 28(1): 154-63.
18. Kokate CK, Purohit AP and Gokhale SB: Pharmacognosy, Nirali Prakash an, Pune, 1998, 23rd Ed.
19. Trease GE and Evans MD: A textbook of Pharmacognosy, Baillier Tindal and Caussel London, 1989 13th Ed.
20. Harborne JB: Phytochemical Methods, A Guide to modern Techniques of Plant Analysis: Chapman and Hall London, 1973.
21. Lowry OH, Roseobrough NJ, Farr AL and Randall RJ: Protein measurement with folin.
22. Zhishen J, Mengcheng T and Jianming W: The determination of flavonoid contents in Mulberry and their scavenging effects on superoxide radicals. Food Chem., 1999; 64: 555-59.
23. Aryal S, Baniya MK, Danekhu K, Kunwar P, Gurung R and Niranjan K: Total Phenolic Content, Flavonoid Content and Antioxidant Potential of Wild Vegetables from Western

Nepal; Plants, 2019; 8: 96.

24. Kumar D, Jamwal A and Madaan R: Estimation of total phenols and flavonoids in selected Indian Traditional plants. Journal of Phamaceutical Technology Research and Management, 2014; 2(1): 77-86.
25. Siddhuraju P and Becker K: Antioxidant properties of various solvent extracts of total phenolic constituents from three different agroclimatic origins of Drumstick tree (Moringa oleifera Lam.) leaves. J Agric Food Chem., 2003; 51: 2144 -155.
26. Kalaichelvi BK and Dhivya SM: Screening of phytoconstituents, UV-VIS Spectrum and FTIR analysis of Micrococca mercurialis (L.). International Journal of Herbal Medicine, 2017; 5: 40-44.