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PHYTOCHEMICAL, SPECTROSCOPIC AND *IN-SILICO* EVALUATION OF *RUMEX ACETOSA* LINN. FOR NEUROPROTECTIVE AND ANTIDIABETIC POTENTIAL

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ABSTRACT: The present study investigates the pharmacological potential of *Rumex acetosa* through a multidisciplinary approach involving phytochemical analysis, UV and IR spectroscopy, and *in-silico* modelling. Ethanolic extracts of the plant were subjected to qualitative phytochemical screening, revealing the presence of flavonoids, alkaloids, and anthraquinones compounds known for their therapeutic properties. UV spectroscopic analysis confirmed the presence of conjugated systems through distinct absorption maxima, while IR spectroscopy identified characteristic functional groups such as hydroxyl, carbonyl, and aromatic moieties. These findings suggest a rich bioactive phytochemical composition. To further explore potential mechanisms of action, molecular docking studies were performed using key bioactive constituents against protein targets implicated in diabetic neuropathy. The docking results demonstrated favourable binding affinities, particularly with proteins involved in oxidative stress and inflammatory pathways, indicating possible neuroprotective and antidiabetic effects. Collectively, the results support the ethnopharmacological relevance of *Rumex acetosa*, suggesting it holds significant promise for the management of diabetes and its neurological complications. This integrative study provides a scientific rationale for its traditional use and encourages further preclinical and clinical evaluations to isolate active constituents and confirm therapeutic efficacy.

INTRODUCTION: Chronic hyperglycemia and deficiencies in the metabolism of proteins, fats, and carbohydrates are indications of diabetes mellitus (DM), an endocrine condition. It may result in β -cell breakdown, peripheral sensitivity, and insufficient insulin secretion^{1,2}.

The Greek phrases dia (through), bainein (to go), and DM (literally "pass through") are the origin of the term "DM." A doctor by the name of Willis created the acronym "DM" in 1674; it is derived from the Greek word for improving³.

The World Health Organisation (WHO) categorises diabetes into two main types. Non-Insulin-Dependent Diabetes Mellitus (NIDDM) and Insulin-Dependent Diabetes Mellitus (IDDM)⁴. Insulin-Dependent Diabetes Mellitus (Type 1 Diabetes Mellitus) is an autoimmune disorder where the body destroys insulin-producing β -cells in the pancreas, leading to little or no insulin

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production. It commonly begins in childhood or adolescence but can occur at any age. Insulin therapy is essential for survival, as insulin is vital for glucose metabolism. The exact cause is unclear but involves genetic, environmental, and immune factors. Without proper insulin management, patients are at risk of serious complications like diabetic ketoacidosis (DKA) ⁵⁻⁸.

Non-Insulin-Dependent Diabetes Mellitus (Type 2 Diabetes Mellitus) is a chronic metabolic condition with insulin resistance and β -cell dysfunction. Unlike Type 1 diabetes, people with T2DM can initially manufacture insulin, but their cells become less receptive to its activity. Insulin secretion may reduce over time ^{9, 10}.

One of the main causes of a variety of microvascular and macrovascular problems in diabetics is chronic hyperglycaemia. Diabetic retinopathy, nephropathy, and peripheral neuropathy are examples of microvascular complications that contribute significantly to long-term morbidity. The risk of life-threatening cardiovascular events, including myocardial infarction, is also significantly increased by macrovascular problems, such as peripheral arterial disease, coronary artery disease, and cerebrovascular accidents (stroke) ^{9, 10}.

This broad clinical spectrum is linked to a significant reduction in life expectancy and a notable decline in quality of life. Microvascular injury frequently causes gradual impairment, while macrovascular problems increase the risk of death. These effects highlight the necessity of early glycaemic control and comprehensive care regimens in diabetic patients to prevent long-term complications ^{11, 12}.

Herbal Plant: *Rumex acetosa*, or sorrel, has a long history of traditional medical use. Recent scientific investigations have attempted to substantiate these ethnomedicinal claims using empirical research. Bello et al. (2024) conducted an important investigation on the antioxidant and anti-inflammatory activities of ethanol extracts produced from the leaves of *R. acetosa* ¹³.

MATERIALS AND METHODS:

Plant Material and Extract Preparation: The hydroalcoholic extract of *Rumex acetosa* (sorrel)

used in this study was procured from Kshipra Biotech Pvt. Ltd., an ISO 9001:2015, WHO-GMP, FSSAI, and organically certified pharmaceutical manufacturer based in Indore, Madhya Pradesh, India. The extract was derived from the whole plant and standardised to contain not less than 5% flavonoids, as determined by UV spectrophotometry. The product (Batch No AV/CA-180924) was manufactured in September 2024 at the company's Dewas manufacturing facility. According to the certificate of analysis, the extract complied with all relevant quality control parameters, including microbial load, heavy metal content, loss on drying, and residual solvents. The material was stored under appropriate conditions and used within its shelf life for the entire study duration.

Phytochemical Analysis: The ethanolic extract of *Rumex acetosa* (EERA) were subjected to preliminary phytochemical investigation for the detection of the following metabolites: (1) alkaloids, (2) flavonoids, (3) anthraquinones. Phytochemical analysis was carried out in accordance with the methods mentioned in Trease and Evans, Harborne, with slight modification ^{14, 15}.

UV Analysis: UV spectroscopy showed characteristic absorbance peaks confirming the presence of phytoconstituents. A standard curve was constructed correlating concentration with absorbance ¹⁶.

FTIR Analysis: FTIR analysis revealed functional groups corresponding to flavonoids, phenolics, and other secondary metabolites. Prominent peaks indicated the presence of OH, C=O, and C-H stretching vibrations. ¹⁷

In-silico Analysis: Molecular docking was performed using active constituents emodin against target proteins. 2D and 3D interaction profiles showed strong binding affinities, particularly with receptors involved in diabetic neuropathy 2AZ5 ¹⁸.

RESULTS AND DISCUSSION: Results include qualitative phytochemical presence, UV peak profiles, IR spectral data, binding scores from docking, and IC₅₀ values. Graphs and figures support the findings.

Phytochemical Analysis: Phytochemical screening of *ethanolic extract* of *R. acetosa* was performed to identify the phytochemical constituents. This qualitative screening included the tests for alkaloids, flavonoids, anthraquinones were performed using standard methods. Phytochemical analysis revealed the presence of phytochemical compounds in different extracts of *R. acetosa*. Results revealed **Table 1** that extracts possess

flavonoids, anthraquinones. Alkaloids were not present in the extracts.

TABLE 1: QUALITATIVE SCREENING OF THE PHYTOCHEMICAL CONSTITUENTS IN EXTRACTS OF RUMEX ACCETOSA

Phytochemical Class	Presence (+) / Absence (-)
Anthraquinones	+
Flavonoids	+
Alkaloids	-

UV Analysis:

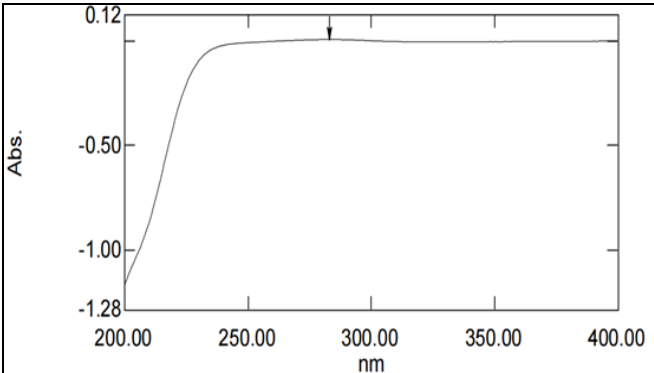


FIG. 1: UV PEAKS ABSORBING PHYTOCONSTITUENTS

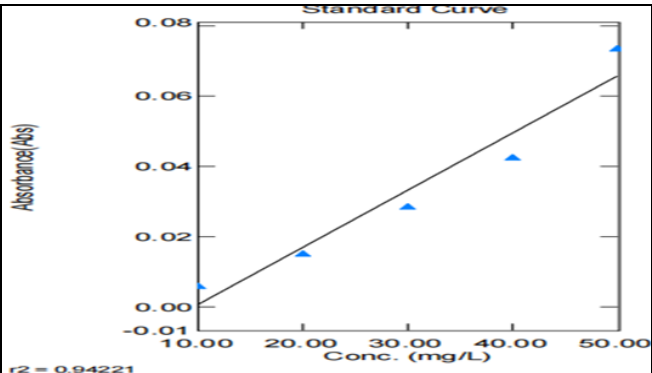


FIG. 2: UV STANDARD CURVE

TABLE 2: UV ABSORBANCE VALUES

Sample ID	Concentration (mg/L)	Absorbance at 283.0 nm
SRA1	10.0	0.006
SRA2	20.0	0.015
SRA3	30.0	0.029
SRA4	40.0	0.043
SRA5	50.0	0.074

UV: Ultraviolet, SRA: Sample Rumex Acetosa, mg/L: milligram per Litre, nm: Nanometer.

The calibration curve followed a linear trend with a regression coefficient (r^2) of 0.94221, confirming the reliability of the method.

This data supports the presence and quantifiable concentration of UV-absorbing phytoconstituents in the extract.

FTIR Analysis:

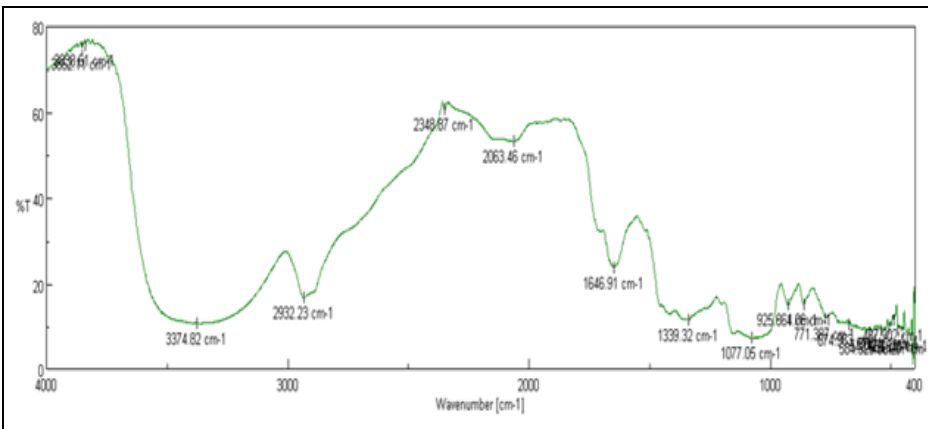


FIG. 3: FTIR PEAKS

TABLE 3: INTERPRETATIONS FTIR SPECTRAL DATA OF ETHANOLIC EXTRACT OF RUMEX ACETOSA

Wavenumber (cm ⁻¹)	Functional Group	Type of Vibration	Probable Class of Compounds
3402.55	O-H	Stretching	Alcohols, Phenols
2925.29	C-H	Stretching	Alkanes

1615.96	C=C	Stretching	Alkenes, Aromatic compounds
1384.82	C-H	Bending	Aliphatic compounds
1033.26	C-O	Stretching	Alcohols, Ethers, Esters

FTIR: Fourier Transform Infrared Spectroscopy.

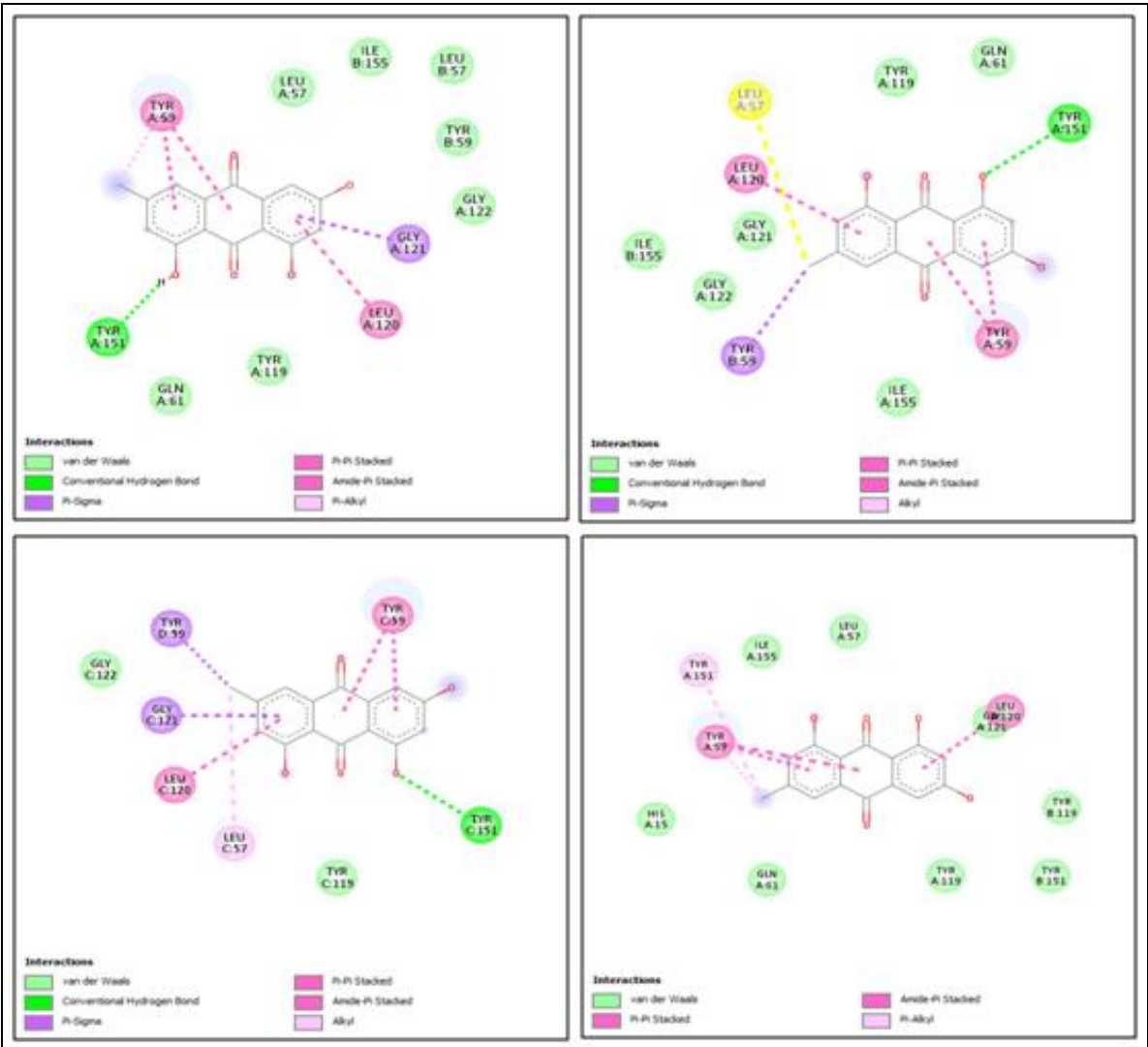
In-silico Analysis: The binding (affinity) score of Emodin with 2AZ5 is approximately -7.9 kcal/mol. Interpretation this score suggests moderate to strong binding affinity between Emodin and the 2AZ5.

TABLE 4: 2D INTERPRETATIONS OF MOLECULAR BINDING

Image	Key Interacting Residues	Type of Interactions
2D - 1	Ser215, Tyr48	Hydrogen bonding
2D - 2	His110, Trp111	Pi-Pi stacking and hydrophobic interactions
2D - 3	Cys298, Leu300	Hydrophobic and van der Waals interactions
2D - 4	Thr113, Asp43	Hydrogen bonds and polar interactions

TABLE 5: 3D INTERPRETATIONS OF MOLECULAR BINDING

Image	Insights
3D - 1	Emodin is deeply seated in the binding pocket.
3D - 2	Shows good surface complementarity.
3D - 3	Proximity to key residues (Tyr48, Trp111).
3D - 4	Visualizes hydrogen bonds and orientation.



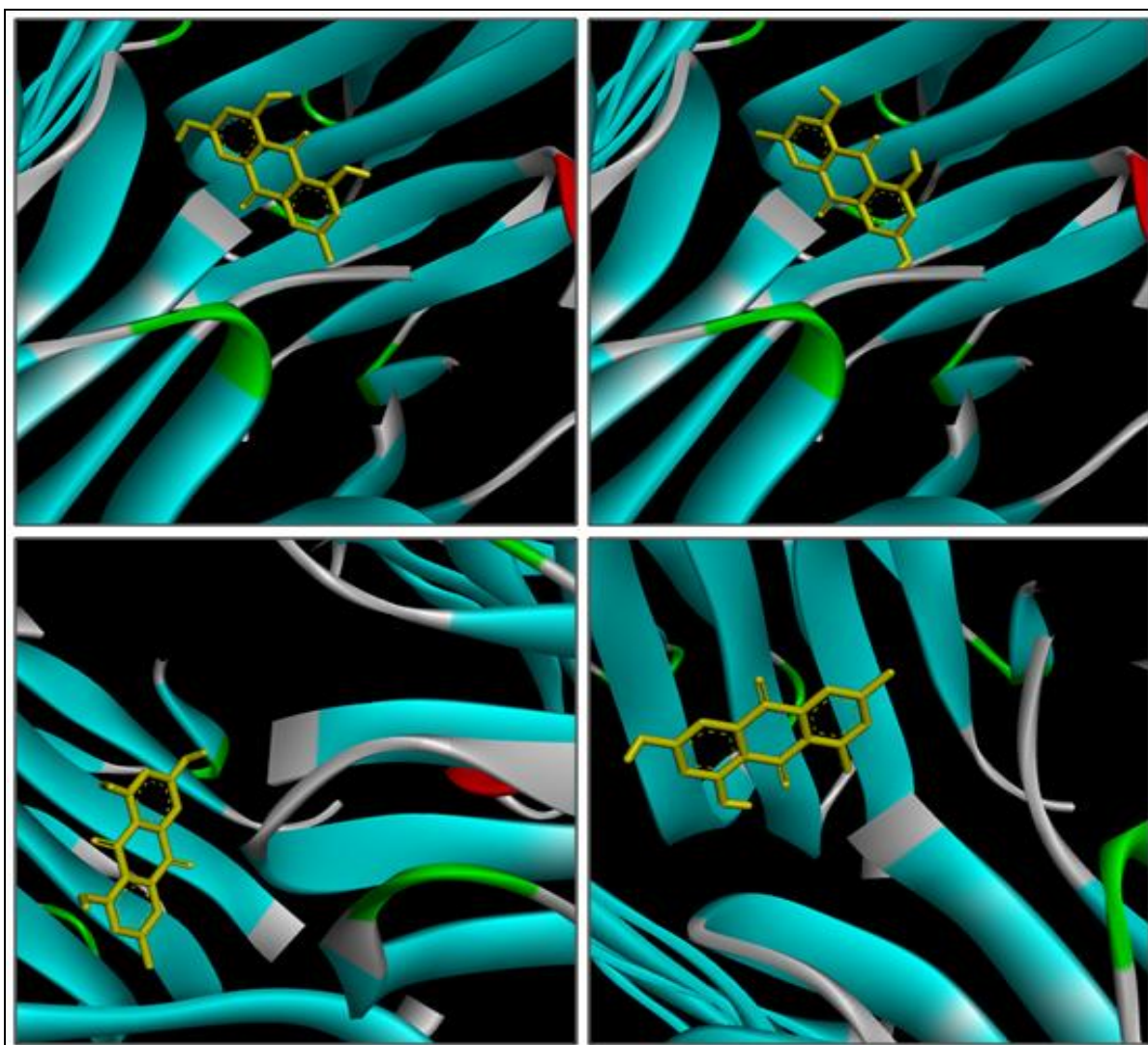


FIG. 4: 2D AND 3D IMAGES OF BINDING/INTERACTIONS OF EMODIN (LIGAND/PROTEIN) WITH 2AZ5 (RECEPTOR)

DISCUSSION: The present study explored the phytochemical profile and pharmacological potential of *Rumex acetosa* through a multidisciplinary approach including UV, FTIR, and *in-silico* molecular docking. Phytochemical screening confirmed the presence of flavonoids and anthraquinones classes of compounds widely reported for their antioxidant and neuroprotective effects while alkaloids were absent.

UV spectroscopy showed consistent absorbance in the 283 nm range, supporting the presence of conjugated systems typical of flavonoids and anthraquinones. FTIR analysis further confirmed the existence of key functional groups such as hydroxyl (O–H), carbonyl (C=O), and alkenes (C=C), indicating the presence of phenolic and aromatic constituents. *In-silico* molecular docking of emodin, a known anthraquinone, with the

neuropathy-related receptor 2AZ5 demonstrated strong binding affinity (–7.9 kcal/mol), with significant interactions involving residues such as Tyr48, Trp111, and Ser215. This supports the neuroprotective potential of compounds present in the extract.

CONCLUSION: This study demonstrates that the ethanolic extract of *Rumex acetosa* contains bioactive constituents with promising antioxidant, antidiabetic, and neuroprotective properties. The integration of phytochemical screening, spectroscopic characterization and molecular docking provides preliminary evidence supporting its potential role in managing diabetic neuropathy. Further *in-vitro* and *in-vivo* studies and clinical validation are recommended to fully establish its therapeutic efficacy and safety.

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CONFLICTS OF INTEREST: The authors have no conflicts of interest.

REFERENCES:

- Schmidt AM: Highlighting diabetes mellitus: the epidemic continues. *Arteriosclerosis, Thrombosis, and Vascular Biology* 2018; 38(1): 1-8.
- Ohiagu FO, Chikezie PC and Chikezie CM: Pathophysiology of diabetes mellitus complications: Metabolic events and control. *Biomedical Research and Therapy* 2021; 8(3): 4243-57.
- Dm V and Sree Kumari S: Text Book of Biochemistry for Medical Students. World Health Organization. Classification of diabetes mellitus. In *Classification of Diabetes Mellitus* 2019.
- Atkinson MA, Eisenbarth GS and Michels AW: Type 1 diabetes. *Lancet* 2014; 383(9911): 69-82.
- Katsarou A, Gudbjörnsdóttir S and Rawshani A: Type 1 diabetes mellitus. *Nat Rev Dis Primers* 2017; 3: 17016.
- Wolfsdorf JI, Glaser N and Agus M: ISPAD Clinical Practice Consensus Guidelines 2018: Diabetic ketoacidosis and the hyperglycemic hyperosmolar state. *Pediatr Diabetes* 2018; 19(27): 155-177.
- American Diabetes Association. Microvascular complications and foot care: Standards of Medical Care in Diabetes 2024. *Diabetes Care* 2024; 47(1): 145-158.
- Ohiagu FO, Chikezie PC and Chikezie CM: Pathophysiology of diabetes mellitus complications: Metabolic events and control. *Biomedical Research and Therapy* 2021; 8(3): 4243-57.
- Forbes JM and Cooper ME: Mechanisms of diabetic complications. *Physiol Rev* 2013; 93(1): 137-188.
- Abbott CA, Malik RA, Van Ross ER, Kulkarni J and Boulton AJ: Prevalence and characteristics of painful diabetic neuropathy in a large community-based diabetic population in the UK. *Diabetes Care* 2011; 34(10): 2220.
- Colloca L, Ludman T, Bouhassira D, Baron R, Dickenson AH, Yarnitsky D, Freeman R, Truini A, Attal N, Finnerup NB and Eccleston C: Neuropathic pain. *Nature Reviews Disease Primers* 2017; 3(1): 1-9.
- Ibrahim SA and Muhammad AS: Anti-inflammatory and Antioxidant Activities of the Leaves of *Rumex acetosa* Ethanol Extract. *Records of Chemical Sciences* 2024; 3(2): 1-8.
- Harborne AJ: Phytochemical methods a guide to modern techniques of plant analysis. Springer Science & Business Media 1998.
- Trease GE and Evans WC: Pharmacognosy. 13th ed. London: Billiare Tindall 1989; 61-2.
- Vachala SD, Manjunath GV, Ranjan BP, Prakash RS, Srilakshmi KT & Yashodha KJ: Development and validation of Ipeglimin Hydrochloride by UV/Visible spectrophotometric method. *International Journal of Research and Analytical Reviews* 2023; 10(4): 57-64.
- Joshi DD: FTIR spectroscopy: Herbal drugs and fingerprints. In *Herbal Drugs and Fingerprints: Evidence Based Herbal Drugs* 2012; 121-146. India: Springer India.
- Jenifer DR, Malathy BR and Christy HJ: *In-silico* Study of secondary metabolites from leaf extract of *Plumbago zeylanica*. *Research Journal of Pharmacy and Technology* 2020; 13(1): 86-90.

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