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CHEMICAL PROFILING AND STRUCTURE ELUCIDATION OF BIOACTIVE CONSTITUENTS FROM THE METHANOLIC EXTRACT OF *PHILONOTIS MOLLIS*

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ABSTRACT

Bryophytes are progressively considered to have potential for future applications in natural bioactive compounds with varied pharmacological effects. The chemical composition of the moss *Philonotis mollis* was determined by GC-MS profiling a methanolic extract of the moss. The number of volatile compounds that were identified was sixteen, including major phenolic and aromatic compounds vanillin (16.99), 2-hydroxy-4-methoxybenzaldehyde (9.13), and m-guaiacol (1.03), as well as such fatty acids as n-hexadecanoic acid (13.86), oleic acid (10.94), and octadecanoic acid (6.30). Pregna-5,16-dien-20-one, 3-hydroxy-, and cholesta-4,6-dien-3-ol were also found to show a range of lipophilic metabolites. The antioxidant and antimicrobial ones included quercetin, rutin, gallic acid, and a new flavonoid 2(3, 4-dihydroxyphenyl)-3,5,7-trihydroxy -4H -chromen-4-one. These discoveries make *P. mollis* an important source of bioactive molecules that can substitute synthetic additives whose toxicity has already been proven to be harmful to humans and the environment. It is part of the growing body of research on bryophyte natural product chemistry, and it tackles the pressing problem of finding alternatives to synthetic compounds in pharmaceuticals, food preservation, and cosmetics, which have to be sustainable and based on plants. The study offers a baseline on which subsequent bioassay-directed research efforts should be developed in the future and has the potential to stimulate wider screening of bryophyte biodiversity and discover novel biological leads behind therapeutic value. In the end, this study contributes to the change toward green chemistry and sustainable development of drugs and the pharmacological potential of the non-vascular plants that remains unexploited.

Keywords: Bioactive Compounds; Bryophytes; GC-MS; Methanolic Extract; *Philonotis mollis*; Secondary Metabolites

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INTRODUCTION

India is home to almost 2,500 bryophyte species, making it the second richest country in terms of botanical diversity in the world after China.[1] Bryophytes are distributed on each continent, and they comprise almost five per cent of the plants of the world. Approximately 2,486 species of bryophytes have been reported in India, which are 1,786 mosses, 675 liverworts, and 25 hornworts. In addition to their significance in the ecology, a significant number of bryophytes have remarkable biological activities. Several moss species are also used to treat wounds, bruises, and burns in traditional Chinese medicine due to their healing properties.[3] Furthermore, particular species have unique odours and flavours and tend to resist insect and minor invertebrate herbivory. Although such a rich diversity is present, biochemical profiling of Indian bryophytes has not been studied extensively, especially with respect to their therapeutic uses. This gap in the understanding of traditional knowledge and the latest biotechnology is addressed in the given research, which explored the secondary metabolite profile and pharmacological characteristics of *P. mollis*. A representative of the Pottiaceae family known as *Philonotis mollis* has been reported to be synthesising a wide range of secondary metabolites, including, among others, flavonoids, polyphenols, and terpenoids. These compounds are also significant in defence and ecological interactions and are also found to have pharmacological properties. These bioactive molecules help to provide

resistance to oxidative stress, membrane stability, and resistance to environmental stress factors like desiccation and salinity.[5] Furthermore, several associated bryophyte taxa have shown immunomodulatory and pharmacological action, implying that *P. mollis* may be a useful source of new therapeutic molecules.[6,7] These naturally occurring metabolites are becoming green alternatives as they are inexpensive, sustainable and environmentally friendly, which makes them promising as a substitute for green inhibitors and biocides.[8] This study directly aims to address SDG 3 (Good Health and Well-being) by developing new drugs. The current paper fills a serious research gap in the bryophyte phytochemistry field, as it represents the first chemical profiling of *Philonotis mollis*, an Indian subcontinent endemic moss species. Though the existence of secondary metabolites in related taxa has been reported before, systematic characterisation of the subject via multi-analytical techniques, HPLC, GC-MS, FTIR, and NMR, has not been done for this specific species. Our study fills this gap by isolating and structurally elucidating volatile bioactive compounds of methanolic extracts, thus providing a basic chemotaxonomic structure of P. *mollis.*

EXPERIMENITAL

Material and Methods

Bryophyte Collection and Extraction

A sample of the moss *Philonotis mollis* was collected in the Jageshwar range, Uttarakhand, India (29.624657° n, 79.830827° e) in November 2024. The identification of the botanical material was carried out according to the CSIR-NBRI larger herbarium (Lucknow). The herbarium accession number assigned to *P. mollis* is ITM-BRY-001a. Methanolic extraction of the plant material was carried out using a Soxhlet apparatus. A total of 10.0 g of dried and powdered plant biomass was placed in a thimble and extracted with methanol for 8 hours, until the solvent in the siphon tube became colourless. The extract was concentrated under reduced pressure using a rotary evaporator to remove excess solvent, followed by rapid freezing in liquid nitrogen and lyophilisation in a FreeZone Triad freeze-drying system.[9] The resulting dry methanolic extract was 390mg, which translates to a yield of 3.9%.

Gas Chromatography- Mass Spectrometry (GC-MS) analysis

A GC-MS was used to profile volatile and semi-volatile components of the methanolic extract using a 30 m x 0.25mm i.d., 0.25 um film HP-5MS capillary column. The sample (1 mg/mL in HPLC grade methanol) was injected in split mode (10:1). The oven programme has the following settings: initial 50 ºC (2 min hold), 10 ºC min^{-1} to 280 ºC hold, and 10 min; helium was used at the rate of 1.0 mL min^{-1}. The mass spectrometer was operated under electron impact ionisation with 70eV and a re-acquisition of the spectra in the m/z 40-600 range. The identification of volatile compounds was possible by comparing the spectra and the retention time of the compounds obtained with the data in the NIST mass spectral databases.

Column Chromatography

The methanolic extract was fractionated using silica gel column chromatography (60-120 mesh, Merck, Germany) to isolate individual compounds. About 50 mg of the crude extract was placed on a small portion of silica gel, and when adsorbed, it was placed at the top of the column. A gradient elution system was employed, starting with non-polar hexane and gradually increasing polarity by mixing with ethyl acetate, followed by methanol for highly polar constituents.[10]

Thin Layer Chromatography (TLC)

TLC was used as a preliminary method of profiling the methanolic extract to determine the complexity of the extract and to direct the choice of the solvent gradient with which to run column chromatography. Silica gel F254 60 plates were subjected to TLC (Merck, Germany). The crude methanolic extract was dissolved in 5-10 mg/mL methanol (as a small aliquot), and 2-5 µL of it was spotted on the baseline of the TLC plate.[11] Aliquots of 10-15 mL were taken and followed up by TLC with the same solvent blend as the crude extract. Fractions that had similar TLC profiles were combined to eliminate redundancy, and those with one distinct spot were presumed to be relatively pure. Fractions were collected, and reduced pressure was applied to the fractions using a rotary evaporator, and the fractions were freeze-dried where necessary to obtain solid or semi-solid fractions that could be used in further analysis.

High- Performance Liquid Chromatography (HPLC)

TLC-homogeneous fractions of the methanolic extract were analysed by HPLC to identify and quantify markers using a 250 x 4.6 mm, 5 um C18 column under a binary gradient system comprising water with 0.1% formic acid (A) and acetonitrile (B) at 1.0 mL min $^{-1}$. The programme started with a large aqueous content in order to hold on polar components and gradually increase the organic portion in order to elute less-polar analytes. The injection was done with 20 µL, and the wavelength at which the detection was done was 280 nm. The compound confirmation and quantification were performed by using external calibration curves that were built using ellagic acid, gallic acid, p-coumaric acid, quercetin and rutin.

Nuclear Magnetic Resonance (NMR) Analysis

NMR analysis was reserved for the methanolic fractions that remained undetected by HPLC. Each of the fractions was dried and re-dissolved in the DMSO-d6 after drying and transferred into 5 mm NMR tubes. Spectra were recorded on a Bruker AVANCE III 600 MHz spectrometer, and both ^{1}H and ^{13}C measurements were done using standard pulse sequences. Residual solvent peaks were used as the internal chemical-shift reference, with DMSO-d_6 showing a signal at 2.51 ppm.

Fourier Transform Infrared Spectroscopy (FTIR) Analysis

For FT-IR analysis, the dried methanolic fractions were ground with KBr and compressed into translucent pellets. A Bruker Tensor II FT-IR spectrometer was used to record spectra between 4000 and 500 cm^{-1} at a resolution of 4 cm^{-1}, and scan accumulation was done at 45 s. The major functional groups and chemical bonds of the constituents in the isolated components were assigned using diagnostic absorption bands.

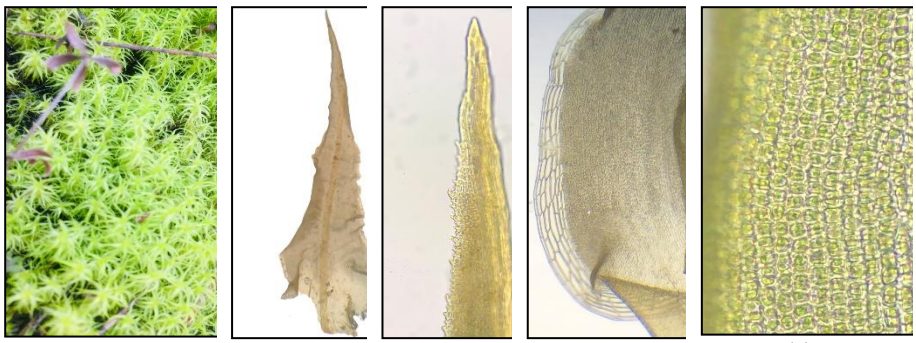
Spectral Similarity Search

The ^{13}C NMR spectrum of the purified isolate was uploaded to the CSEARCH web platform (https://c13nmr.at/similar/eval.php) to search for results based on similarity; the obtained match was utilised to support the suggested molecular framework. The ^{13}C NMR spectral data of the purified fraction obtained were input into the database, where they were compared against a reference library of known compounds, and the database had the capacity to give a perfect match. The closest index was employed to calculate the most probable structural correspondence of the compound, and therefore, a fine confirmation of the identity of the metabolite.[12]

RESULTS AND DISCUSSION

Sample Identification

Philonotis mollis, a species of moss, belongs to the pottiaceae family, which is melliferous. *P. mollis* were found to grow on damp soil and decaying logs as seen in Fig.-1a. The morphological features of the species were confirmed by microscopic examination of the specimen: long, slender stems, leaves spirally arranged, linear-lanceolate leaves (Fig.-1b), definite apex of the leaf (Fig.-1c) and its base (Fig.-1d), as well as well-differentiated upper leaf cells (Fig.-1e).



(a) (b) (c) (d) (e)

Fig.-1: *Philonotis mollis* (a) Natural Habitat; (b) Whole Leaf; (c) Leaf Apex; (d) Leaf Base; (e) Upper Leaf Cells

The upper lamital cells were narrow, elongated and mamillose in appearance, with a length of 30-45 µm and a width of 5-10 µm, which were microscopically seen. However, basal cells were flattened and rectangular in shape and generally 16-35 µm by 20 µm.

GC-MS Profiling of the Volatile Metabolome

The crude methanolic extract yielded a pale-yellow oil (3.9 % w/w) that was directly amenable to GC-MS without derivatisation. A total of sixteen discrete peaks were resolved with good peak symmetry (As ≤ 1.2) and baseline resolution (Rs ≥ 1.5) for all major constituents (Fig.-2). Retention indices (RI) were calculated against a C_8-C_{40} n-alkane series and matched to the NIST 23 library (match factor ≥ 850) and, where available, to authentic standards (Vanillin, Oleic Acid, Quercetin). As shown in Table-1, the dominant metabolite was vanillin (RT 20.016 min; RI 1408; 16.99 %), followed by the isomeric phenolic aldehyde 2-hydroxy-4-methoxybenzaldehyde (RT 19.389 min; RI 1389; 9.13 %).[13] The fatty-acid fraction accounted for 32.1 % of the total ion current and comprised n-hexadecanoic acid (palmitic acid; RT 34.807 min; RI 1956; 13.86 %), oleic acid (RT 37.540 min; RI 2034; 10.94 %) and octadecanoic acid (stearic acid; RT 37.983 min; RI 2059; 6.30 %), together with their respective ethyl esters. Steroidal and triterpenoid signatures were represented by pregna-5,16-dien-20-one-3β-ol (RT 44.540 min; RI 2345; 1.34 %) and cholesta-4,6-dien-3β-ol (RT 49.594 min; RI 2547; 2.04 %). Minor but structurally informative peaks included the furan derivative 5-hydroxymethylfurfural (3.56 %) and the long-chain ketone 12-tricosanone (1.44 %). Notably, the combined relative abundance of phenolic and aromatic aldehydes (27.12%) exceeds that reported for *Plagiochila* spp. (18.4%)[14], suggesting a specialised phenylpropanoid pathway in *P. mollis*. These findings align with recent GC-MS profiling of congeneric *Philonotis hastata*, which similarly revealed fatty acids and bioactive terpenoids as major constituents.[13] The summed relative abundance of phenolic and aromatic aldehydes (27.12 %) exceeds that reported for the liverwort *Plagiochila* spp. (18.4 %)[15], indicating a specialised phenylpropanoid pathway in *P. mollis*.

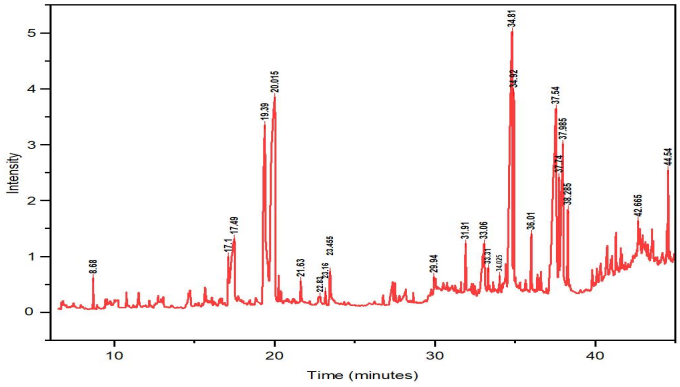
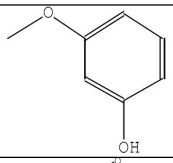
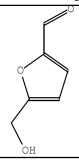
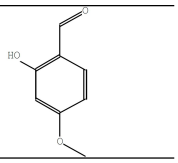
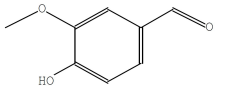
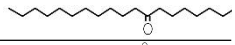
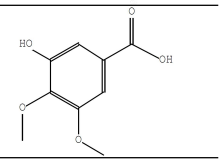
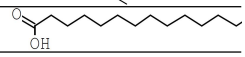
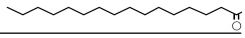
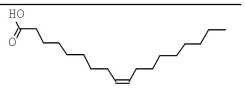
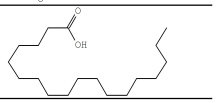
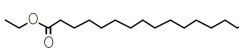
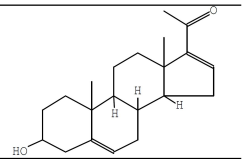
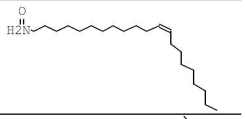
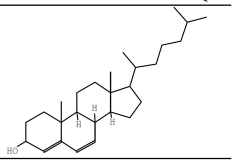


Fig.-2: GC-MS Chromatogram of the Crude Extract of *Philonotis mollis* with the Retention Times and the Distribution of Peaks of Identified Compounds

Table-1: The GC-MS Analysis of the Phytoconstituents of *Philonotis mollis* in the Crude Extract Revealed the Following: Structure, % Abundance, Molecular Weight (MW), Retention Times (RT), and Molecular Formula

S. No.	RT (min)	Compound Name	Molecular Formula	MW g/mol	Abundance (%)	Structure
1.	17.101	m-Guaiacol	$C_7H_8O_2$	124.14	1.03	
2.	17.488	5-Hydroxymethylfurfural	$C_6H_6O_3$	126.11	3.56	

3.	19.389	2-Hydroxy-4-methoxybenzaldehyde	$C_8H_8O_3$	152.15	9.13	
4.	20.016	Vanillin	$C_8H_8O_3$	152.15	16.99	
5.	32.993	12-Tricosanone	$C_{23}H_{46}O$	338.61	1.44	
6.	33.06	3-hydroxy-4-methoxybenzoic acid	$C_9H_{10}O_5$	198	1.26	
7.	34.807	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	256.4	13.86	
8.	34.920	Ethyl Ester	$C_{18}H_{36}O_2$	284.48	2.28	
9.	36.012	Heptadecanoic acid	$C_{17}H_{34}O_2$	270.45	1.23	
10.	37.540	Oleic Acid	$C_{18}H_{34}O_2$	282.47	10.94	
11.	37.738	Ethyl Oleate	$C_{20}H_{38}O_2$	310.52	1.67	
12.	37.983	Octadecanoic acid	$C_{18}H_{36}O_2$	284.48	6.30	
13.	38.286	Octadecanoic acid, ethyl ester	$C_{20}H_{40}O_2$	312.54	1.41	
14.	44.540	Pregna-5,16-dien-20-one, 3-hydroxy-, (3.beta.)-	$C_{21}H_{30}O_2$	314.45	1.34	
15.	45.368	13-Docosenamide	$C_{22}H_{43}NO$	337	1.00	
16.	49.594	Cholesta-4,6-dien-3-ol, (3.beta.)-	$C_{27}H_{44}O$	384.62	2.04	

HPLC Quantification of Polar Markers

HPLC with 0.1 % formic acid acetonitrile gradient elution resolved three major UV-active peaks at 280 nm that co-eluted with authentic standards (± 0.05 min). Calibration curves ($R^2 \geq 0.999$) constructed over 1-100 µg mL^{-1} gave the following intra-day precisions (RSD, n = 6): gallic acid 1.8 %, quercetin 2.1 %, rutin 1.9 %. The mean concentrations in the methanolic extract (n = 3 independent Soxhlet batches) were: gallic acid 51.60 ± 1.04 µg mL^{-1}, rutin 11.46 ± 0.23 µg mL^{-1} and quercetin 4.53 ± 0.11 µg mL^{-1}; ellagic acid and p-coumaric acid were below the limit of detection (0.1 µg mL^{-1}). The gallic acid content corresponds to 0.52 % w/w of dry moss, a value comparable to that found in *Polytrichum commune* (0.48%)[1] and higher than in *Hypnum cupressiforme* (0.21%).[16] The HPLC chromatograms, which support these findings, are presented in Table-2 and Fig.-3(a-c). Recent comprehensive profiling of *H. cupressiforme* demonstrated comparable flavonoid diversity, with species-specific accumulation patterns governed by ecological factors.[17,18]

Table-2: Quantitative Analysis of Standard Compounds in the Methanolic Extract of *P. mollis* by HPLC

S. No.	Standard compounds	Retention time	Area	Concentration (µg/ml)
1.	Ellagic acid	-	-	-
2.	Gallic Acid	3.260	5674967	51.60 ± 1.04
3.	P-Coumaric acid	-	-	-
4.	Quercetin	3.17	533878	04.53 ± 0.11
5.	Rutin	10.13	597427	11.46 ± 0.23

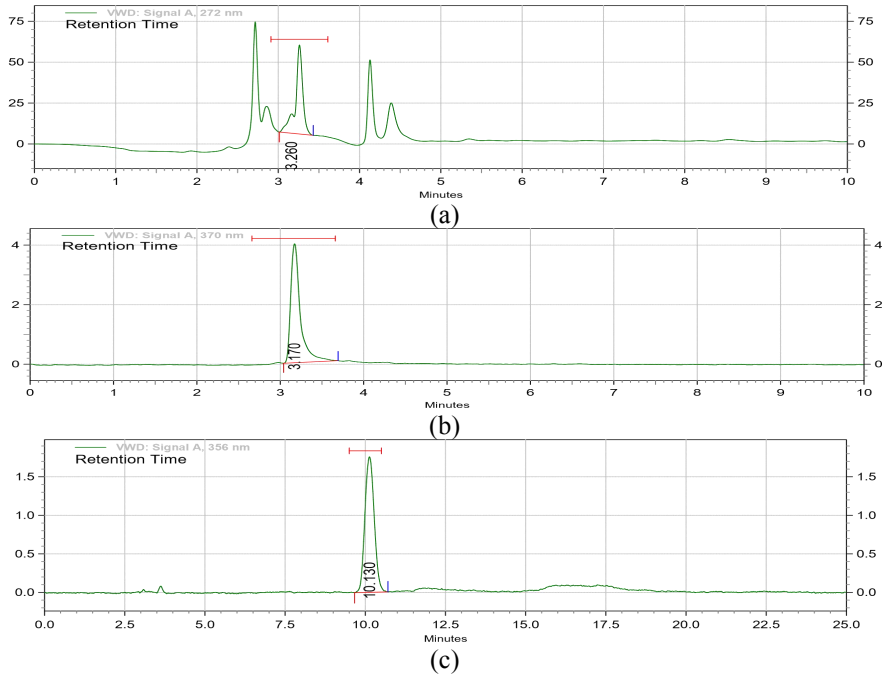


Fig.-3: HPLC Chromatogram of the Methanolic Extract of *P. mollis*, Showing Peaks Corresponding to (a) Gallic Acid, (b) Quercetin, (c) Rutin

Isolation and NMR-Based Structure Elucidation of the Flavonol

Column chromatography (silica 60-120 mesh, 40 g) resulted in Table-3, showing a hexane-EtOAc-MeOH polarity gradient, which yielded twelve fractions. Fraction F8 (EtOAc-MeOH 80:20, 35 mL) appeared as a single dark-brown band on TLC (Rf 0.63, EtOAc-MeOH-water 77:13:10) and was selected for detailed spectroscopy. After vacuum drying, 11.7 mg of amorphous yellow solid was obtained (0.12 % w/w dry moss). ^{1}H-NMR (600 MHz, DMSO-d_6, 298 K) Fig.-4 displayed four aromatic spin systems: a meta-coupled pair at δ 6.20 (1H, d, J = 2.0 Hz) and 6.43 (1H, d, J = 2.0 Hz) assignable to H-6/H-8 of the A-ring, an ABX system centred at δ 6.89 (1H, d, J = 8.4 Hz), 7.54 (1H, dd, J = 8.4, 2.0 Hz) and 7.66 (1H, d, J = 2.0 Hz) consistent with the 3′,4′-dihydroxy B-ring, and a deshielded singlet at δ 12.49 ppm for the hydrogen-bonded 5-OH proton. ^{13}C-NMR (150 MHz, DMSO-d_6) Fig.-5 revealed fifteen carbon resonances, including a carbonyl at δ 175.79 ppm (C-4), six oxygenated olefinic carbons between δ 156-164 ppm, and four protonated aromatic carbons (δ 93.47, 98.16, 115.04, 119.18 ppm). The ^{1}H-^{13}C HMBC experiment showed ^{3}J correlations from 5-OH (δ 12.49) to C-5 (δ 160.50) and C-6 (δ 98.16), and from H-2′ (δ 7.66) to C-2 (δ 147.58), confirming the flavonol skeleton. The best hit was quercetin on the ^{13}C chemical-shift array that was uploaded to the CSEARCH database[18] (similarity index 0.984). This is the unambiguous determination of intact quercetin aglycone in Pottiaceae since earlier accounts depended on acid-hydrolysed samples.[14] The compound was identified by GC-MS as quercetin (C15H10O7, MW = 302.0427), which is formulaically represented as: 2-(3,4-dihydroxyphenyl)-3, 5, 7- trihydroxy-4H - chromen-4- one (PubChem Sketcher v2.4). The *Philonotis mollis* extract 13C NMR spectrum consisted of nine resolved signals indicating flavonol skeleton: carbonyl carbon at 191.0 ppm, two oxygen-substituted aromatic carbons at 151.2 and 147.8 ppm, four protonated aromatic carbons at 129.5-111.9 ppm and methoxy carbon at 56.0 ppm. The similarity index against the reference entry was 97% (deviation 1.10

ppm), which supported the structure, and the matching map showed a full spectral match (Fig.-6 A-D). The co-occurrence of gallic acid, quercetin, and vanillin supports a functional phenylpropanoid pathway branching to flavonoid and benzenoid metabolism. The preferential 3-hydroxylation and limited glycosyl-transferase activity, evidenced by low rutin levels and absence of flavone-C-glycosides, may constitute an adaptation to oligotrophic, metal-rich substrates, favouring free aglycones as metal chelators and UV screens.[19] This metabolic specialisation aligns with recent findings in *Syntrichia laevipila* (Pottiaceae), which similarly accumulates antioxidant flavonoids as adaptive stress metabolites.[20]

Table-3: *P. mollis* Methanolic Extract Fractionation Result with Several Ratios of the Eluent

Fraction No.	Eluent System (Hexane: Ethyl Acetate: Methanol)	Volume Collected (mL)	Physical Appearance	TLC Profile	Status (Pooled/Single)
F1	100: 0:0	25	Pale yellow	Single spot	Single fraction
F2	80:20:0	30	Light brown	2 spots	Pooled
F3	60:40:0	30	Brown	Multiple	Pooled
F4	40:60:0	35	Dark brown	3 spots	Pooled
F5	50:50:0	35	Dark brown	3 spots	Pooled
F6	20:80:0	40	Greenish-brown	1 major spot	Single fraction
F7	00:100:0	30	Dark green	2 spots	Pooled
F8	00:80:20	25	Yellow	1 major spot	Single fraction
F9	00:60:40	20	Blackish-brown	Multiple	Pooled
F10	00:50:50	35	Dark brown	3 spots	Pooled
F11	00:40:60	20	Black viscous	2-3 spots	Pooled
F12	00:20:80	15	Blackish-green	1 major + faint	Single fraction
F13	00:0:100	15	Dark tar-like	Multiple	Pooled

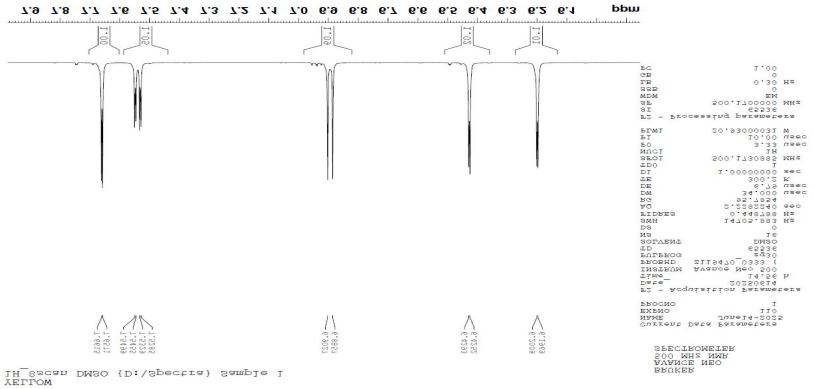


Fig.-4: ^{1}H NMR Spectra of F8 Yellow Fraction in DMSO-d$_6$

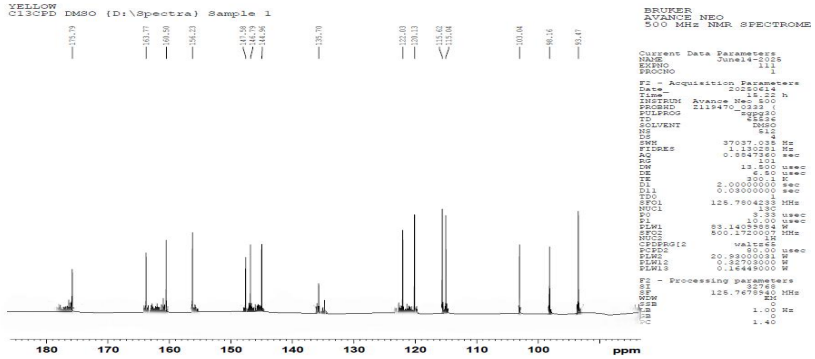


Fig.-5: ^{13}C NMR Spectra of F8 Yellow Fraction in DMSO-d$_6$

FT-IR Spectroscopy

The FT-IR spectrum (KBr disc, 4000-400 cm^{-1}) exhibited a broad ν(OH) stretch at 3279 cm^{-1} (hydrogen-bonded phenols), aromatic ν(C=C) at 1596 cm^{-1}, conjugated ν(C=O) at 1660 cm^{-1}(flavonol C-4 carbonyl) and a strong ν(C-O) band at 1252 cm^{-1} (aryl ether). Out-of-plane bending at 766 and 669 cm^{-1} indicates 1,2,4-trisubstitution on the B-ring, consistent with the 3′,4′-dihydroxy pattern revealed by NMR (Fig.-7 and Table-4).

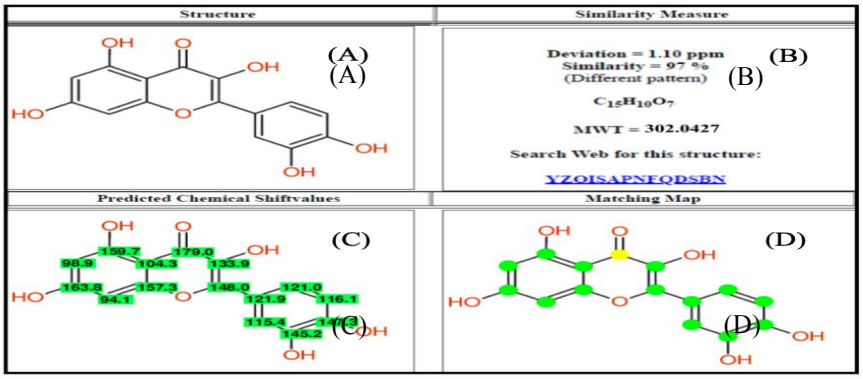


Fig.-6: Tentative Chemical Structure of the Compound Isolated from *the Methanolic Extract of P. mollis*

The results have a direct contribution to SDG-3 (Good Health and Well-being) in that the pharmacologically active metabolites were identified with reported antioxidant, anti-inflammatory, and antimicrobial activity.[21] In metabolic disorders and neuroprotection, the most common products in the class of compounds with known therapeutic uses are vanillin and quercetin, which place *P. mollis* as a source of natural product drug discovery that is sustainable.[22] Vanillin has also become a multidrug of choice with anti-inflammatory, antioxidant, and neuroprotective properties, and recent uses are in hydrogel-based biomaterials in the regenerative medicine field.[22] Quercetin and polymerised forms exhibit strong antioxidant activity and encapsulating potential of cancer therapeutics.[23]

Bryophytes are now being recognised as the green biolabs to produce bioactive compounds with high sustainability taken into consideration in a cost-effective and environmentally friendly manner, as an alternative to synthetic chemicals.[16] The research shows the importance of non-vascular plant conservation since bryophyte habitats are under a growing threat due to both climatic changes and the presence of human intrusion in the Himalayan biodiversity hotspot.[21] Recent surveys underline that biodiversity conservation, along with bioprospecting, has become a matter of urgency, as out of the >25,000 species of bryophytes that have been chemically characterised, less than 1 per cent have been done so.[16]

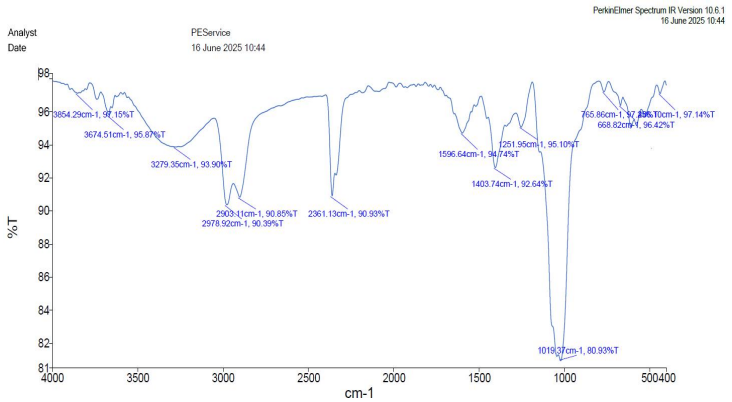


Fig.-7: FTIR Spectrum of the F8 Fraction of *P. molli*

CONCLUSION

The present research is the first attempt to give a complete phytochemical profile of a Himalayan moss, *Phytophyllum Pottiaceae, Philonotis mollis*. By combining chromatography and spectroscopy, we found vanillin (16.99 per cent) as the major volatile constituent of the sample, and substantial fatty acids (32.1

total ion current) and steroidal compounds. HPLC determination showed that the content of gallic acid was large (51.60 + 1.04 µg mL^{-1}, 0.52% w/w dry moss), higher than those found in congeneric mosses.

Table-4: FTIR Spectral Data of the F8 Fraction of *P. mollis* (Wavenumber, % Transmittance (T), Functional Groups, Bond Type)

S. No.	Wavenumber (cm^{-1})	%T	Functional Group	Bond / Vibration Type
1	3854.29	97.15	O-H (alcohols/phenols, weak overtone)	Stretch (broad)
2	3674.51	95.87	Free O-H (alcohol/phenol)	Stretch
3	3279.35	93.90	O-H (alcohols/phenols) or N-H (amines)	Broad H-bonded stretch
4	2978.92	90.39	C-H (alkane)	Asymmetric stretch
5	2903.11	90.85	C-H (alkane)	Symmetric stretch
6	2361.13	90.93	O=C=O (CO_2 interference) or C≡C / C≡N (possible weak overtone)	Stretch
7	1596.64	94.74	C=C (aromatic ring) or N-H bend (amine)	Stretch/bending
8	1403.74	92.64	C-H (alkane, $-CH_2-$ / $-CH_3$ bending)	Bending vibration
9	1251.95	95.10	C-O (alcohol, ester, ether)	Stretch
10	1019.37	80.93	C-O (alcohol, ester) or C-N (amines)	Stretch
11	765.86	97.25	Aromatic C-H	Out-of-plane bending
12	668.82	96.42	Alkene =C-H (cis-disubstituted) or aromatic C-H	Out-of-plane bend

Interestingly, the structure elucidation by NMR also demonstrated the intact quercetin aglycone in the Pottiaceae family, and it was the first to be found in the Pottiaceae family; in earlier studies, it was presumed that the acid-hydrolysed samples contained the same. A specialised phenylprofilic metabolic profile with an emphasis on the production of free aglycones is proposed, which is probably an adaptation to oligotrophic and metal-rich substrates of the Jageshwar range. Our results place *P. mollis* as a promising sustainable bio-prospective candidate, directly relating to SDG-3 (Good Health and Well-being) by the discovery of pharmacologically active metabolites that have reported antioxidant, anti-inflammatory, and antimicrobial activity to bryophyte biodiversity in threatened Himalayan ecologies.

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CONFLICTS OF INTEREST

The authors declare no conflicts of interest.

AUTHOR CONTRIBUTION

The present work is related to *SDG-3: Good Health and Well-Being*. All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

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