

Molecular Docking and Anti-tubercular potential of bioactive compounds from *Houttuynia Cordata*

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Abstract-Tuberculosis (TB), caused by *Mycobacterium tuberculosis*, remains a major global health challenge due to increasing drug resistance and limitations of existing therapies. The present study investigated the anti-tubercular potential of bioactive constituents of *Houttuynia cordata*. The methanolic extract of *H. cordata* (FMEM) was subjected to preliminary phytochemical and spectroscopic/chromatographic characterization. Selected phytoconstituents were further evaluated by molecular docking against potential *M. tuberculosis* protein targets to assess their binding affinity and interaction profiles. The selected compounds exhibited favorable interactions with the investigated targets, indicating their potential for anti-tubercular drug discovery. The *in vitro* anti-tubercular activity of FMEM was evaluated against *M. tuberculosis* H37Rv using the Microplate Alamar Blue Assay (MABA) at concentrations ranging from 100 to 0.2 µg/mL. The extract showed susceptibility at 100 µg/mL, while no detectable inhibition was observed at lower tested concentrations. Accordingly, the minimum inhibitory concentration (MIC) of FMEM was reported as 100 µg/mL. Rifampicin, isoniazid, and pyrazinamide were used as reference drugs. Overall, the findings provide preliminary evidence for the anti-tubercular potential of *H. cordata* and its bioactive constituents, warranting further experimental validation.

Index Terms-Anti-tubercular activity, *Houttuynia cordata*, *Mycobacterium tuberculosis*, MABA, MIC, molecular docking, phytoconstituents.

I. INTRODUCTION

Tuberculosis (TB), caused by *Mycobacterium tuberculosis*, remains a major global health concern, particularly due to the emergence of drug-resistant strains and the limitations of prolonged anti-tubercular therapy. This has increased the need to explore new and effective therapeutic agents from natural sources. Medicinal plants are an important source of bioactive compounds with diverse pharmacological properties and may provide promising leads for drug discovery.

Houttuynia cordata Thunb., commonly known as fish mint or chameleon plant, belongs to the family Saururaceae. It is a perennial herb widely distributed in parts of South and Southeast Asia and has a long history of traditional medicinal use. Different parts of the plant have been traditionally used for conditions associated with inflammation and infection. Phytochemical investigations have reported the presence of flavonoids, phenolic compounds, alkaloids, volatile oils, and other bioactive constituents. Flavonoids such as quercitrin and related compounds have attracted considerable interest because of their reported antimicrobial and antioxidant properties.

The biological activities of these phytoconstituents suggest that *H. cordata* may serve as a potential source of compounds with anti-tubercular activity. The Microplate Alamar Blue Assay (MABA) is a useful *in vitro* method for evaluating the inhibitory activity of test extracts against *M. tuberculosis*. Molecular docking can further provide insights into the possible interactions of selected phytoconstituents with relevant mycobacterial protein targets.

Therefore, the present study aimed to evaluate the anti-tubercular activity of the methanolic extract of *H. cordata* against *M. tuberculosis* H37Rv using MABA and to investigate the binding potential of selected phytoconstituents through molecular docking studies.^[1,2,3]



Figure 1: *Houttuynia cordata* plant.^[14]

II. MATERIALS AND METHODS

1. Plant Material and Preparation

Houttuynia cordata was collected from Mahadevapura, Bengaluru. The collected plant material was shade-dried for 4 days, powdered, and subjected to extraction. The loss on drying was determined as 7.57%.^[3]

2. Extraction

The powdered plant material (10 g) was extracted using Soxhlet extraction. For methanolic extraction, 300 mL methanol was used as the solvent and extraction was carried out at 70–100°C for 7–8 h. The extract was concentrated, dried, weighed, and stored for further analysis. The methanolic extract obtained was 1.63 g, corresponding to a reported yield of 16.30%.^[5]

3. Preliminary Phytochemical Screening

The extract was subjected to standard qualitative phytochemical screening for the detection of major secondary metabolites. Alkaloids, glycosides, flavonoids, saponins, carbohydrates, tannins, and phenolic compounds were reported in the extract.^[5,6]

4. Molecular Docking Study

Molecular docking was performed to investigate the interaction of selected phytoconstituents with *M. tuberculosis* protein targets. The selected targets were PDB IDs 4QXM (InhA), 5HJ7 (MurI), and 4NNH (RpsA).

Protein structures were cleaned and prepared by removing water molecules, heteroatoms, nucleic acids, and co-crystallized ligands, followed by addition of polar hydrogens and Kollman charges. Selected ligands were prepared using ACD/ChemSketch and AutoDock tools, with hydrogen addition, Gasteiger charge assignment, and rotatable-bond definition before conversion to PDBQT format.

Docking was carried out using AutoDock Tools 1.5.7, and the docked complexes were analyzed using BIOVIA Discovery Studio Visualizer v21.1.0.20.29. The docking workflow included target selection, protein and ligand preparation, grid generation, docking, and analysis of binding interactions.^[7]

5. In Vitro Anti-tubercular Activity

The methanolic extract of *H. cordata* (FMEM) was evaluated against *Mycobacterium tuberculosis* H37Rv using the Microplate Alamar Blue Assay (MABA). The extract was tested at concentrations ranging from 100 to 0.2 µg/mL, with rifampicin, isoniazid, and pyrazinamide used as reference drugs. The minimum inhibitory concentration (MIC) was determined based on the assay response.^[8]

III. RESULTS AND DISCUSSION

Extraction Yield

The extraction yield of *Houttuynia cordata* varied according to the solvent used. Among the evaluated extracts, methanol showed the highest extraction yield (16.30%), followed by hydroalcoholic methanol: water (70:30) (11.50%) and ethanol (9.17%). Petroleum ether and chloroform produced considerably lower yields of 1.30% and 1.00%, respectively. The extractions were performed at 70–80°C for 7–8 h. The highest yield obtained with methanol suggests efficient extraction of the polar and moderately polar constituents present in the plant material.

Extracting solvent	Temperature (°C)	Duration (h)	Yield (%)
Methanol	70–80	7–8	16.30
Methanol: Water (70:30)	70–80	7–8	11.50
Ethanol	70–80	7–8	9.17
Petroleum ether	70–80	7–8	1.30
Chloroform	70–80	7–8	1.00

Table 1. Percentage yield of different extracts of *Houttuynia cordata*

Preliminary Phytochemical Screening

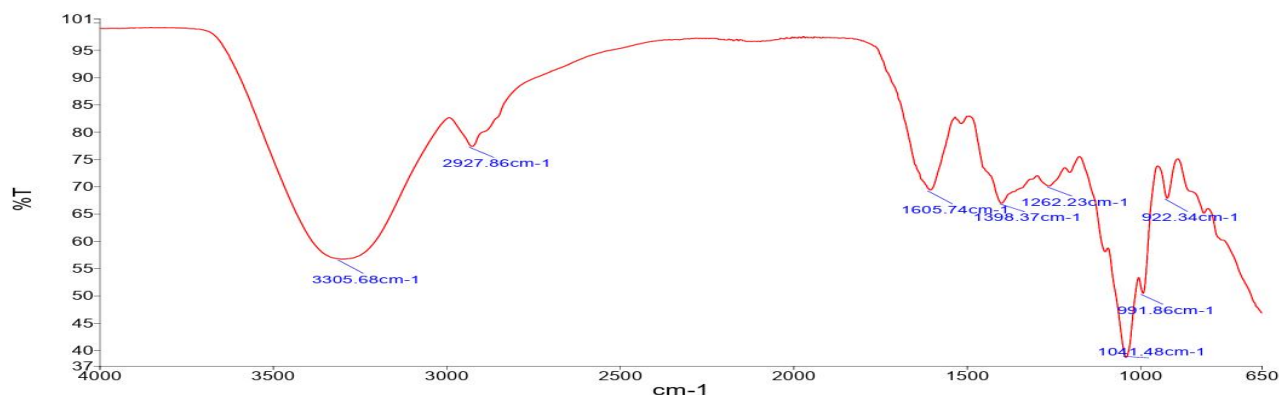
Preliminary phytochemical screening of the *H. cordata* extract demonstrated the presence of several classes of secondary metabolites. **Alkaloids, saponins, glycosides, carbohydrates, phenolic compounds, and flavonoids** were detected, whereas **tannins were absent**. The presence of flavonoids and phenolic constituents is particularly noteworthy because these classes comprise numerous biologically active compounds and may contribute to the pharmacological potential of the extract.

Phytochemical constituent	Result
Alkaloids	Present
Saponins	Present
Glycosides	Present
Carbohydrates	Present
Phenolic compounds	Present
Flavonoids	Present
Tannins	Absent

Table 2. Preliminary phytochemical screening of *Houttuynia cordata* extract

FTIR Analysis

FTIR analysis was performed to identify characteristic functional groups present in the investigated sample. The spectrum exhibited absorption bands at **3305.68, 2927.86, 1398.37, 1262.23, and 1041.48 cm^{-1}** , corresponding to O–H, COOH, N–O, C–H, and C–N functional groups, respectively. The observed spectral profile indicates the presence of diverse functional groups that may be associated with the phytochemical constituents of *H. cordata*.

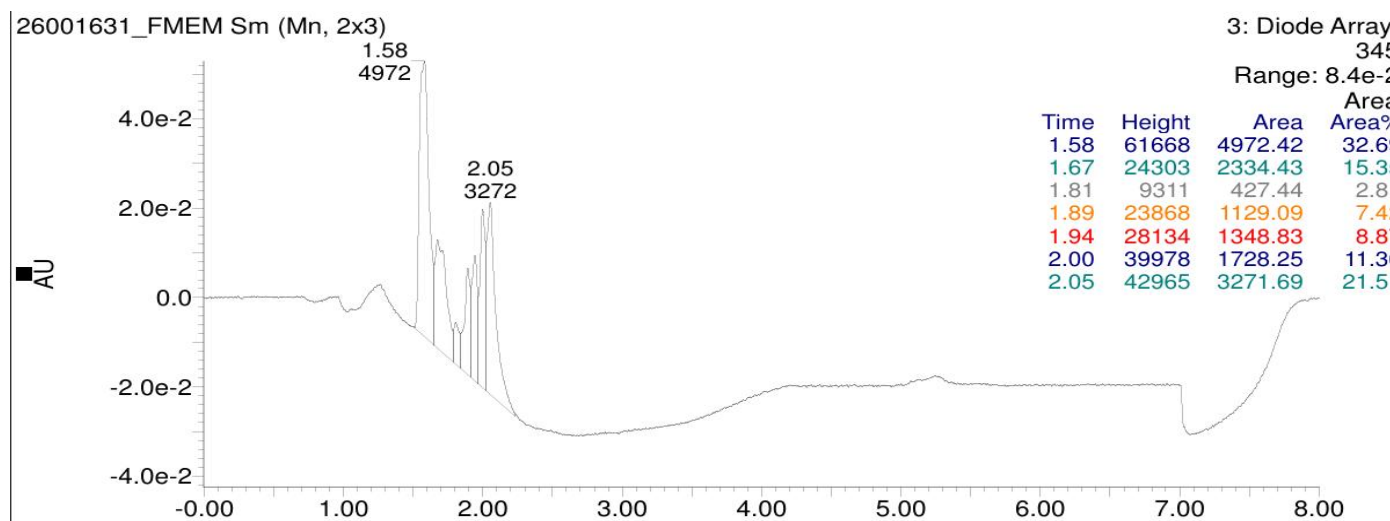


Functional group	Standard range (cm^{-1})	Observed frequency (cm^{-1})
O–H	3500–3200	3305.68
COOH	3300–2500	2927.86
N–O	1400–1290	1398.37
C–H	1300–1000	1262.23
C–N	1250–1020	1041.48

Table 3. FTIR spectral interpretation

LC–MS Analysis

LC–MS analysis generated chromatographic retention-time profiles along with electrospray ionization (ES^+ and ES^-) profiles of the investigated sample. These analytical profiles provided supporting information for the characterization of constituents present in the extract.

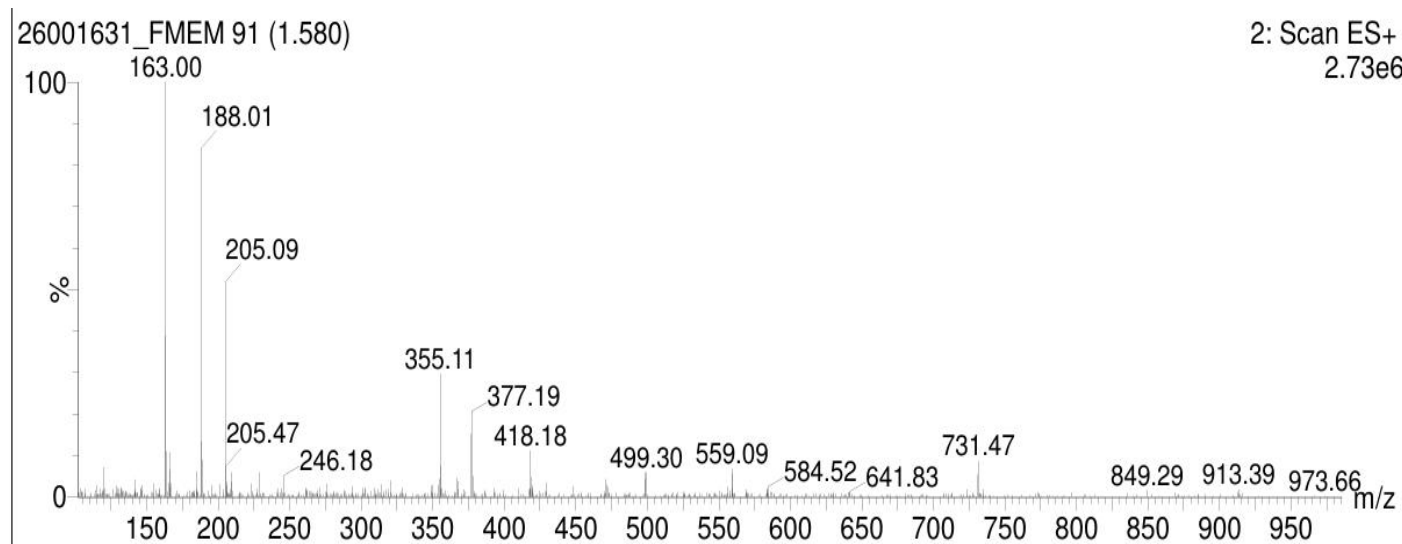


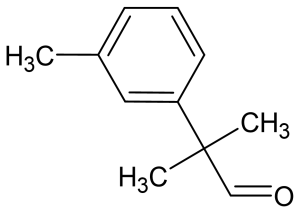
CONSTITUENTS	TIME (min)	HEIGHT (μAU)	AREA (μAU.min)	AREA%
CHLOROGENIC ACID	1.58	616668	4972.42	32.69
M-TOLYL DIMETHYL ACETALDEHYDE	1.67	24303	2334.43	15.35
RUTIN	1.81	9311	427.44	2.81
HYPEROSIDE	1.89	23868	1129.09	7.42
HOULTYUNOSIDE	1.94	28134	1348.83	8.87
QUERCETIN	2.00	39978	1728.25	11.36
QUERCITRIN	2.05	42965	3271.69	21.51

Table 4. Quantification data

Mass Spectrometric Analysis

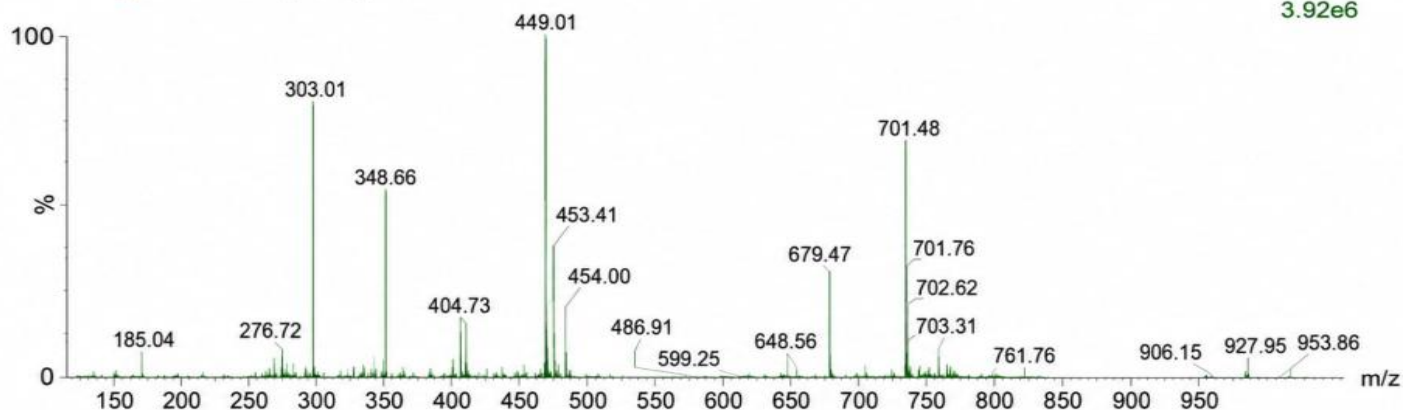
Mass spectrometric analysis produced molecular-ion and fragment-ion data for the detected constituents. The recorded molecular weights ranged from **162 to 610**, with corresponding molecular-ion and fragment peaks observed in both positive- and negative-ionization modes. These data supported the characterization of multiple constituents associated with the investigated *H. cordata* extract.

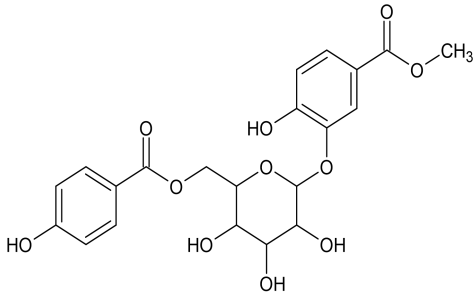


	Molecular weight	162
	Molecular ion peak	163
	Fragment	118

26001631_FMFM 115 (1.997)

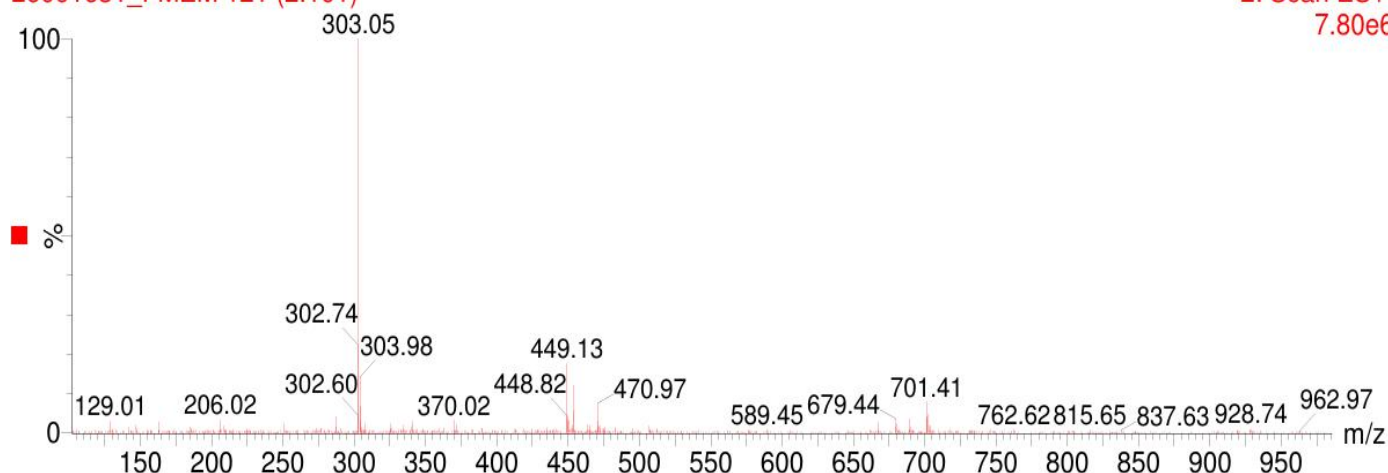
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3.92e6

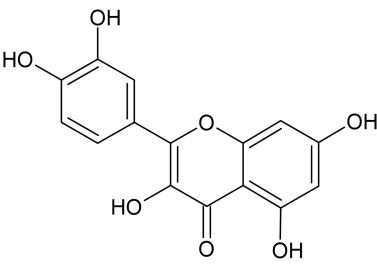


	Molecular weight	450
	Molecular ion peak	499
	Fragment	404

26001631_FMFM 121 (2.101)

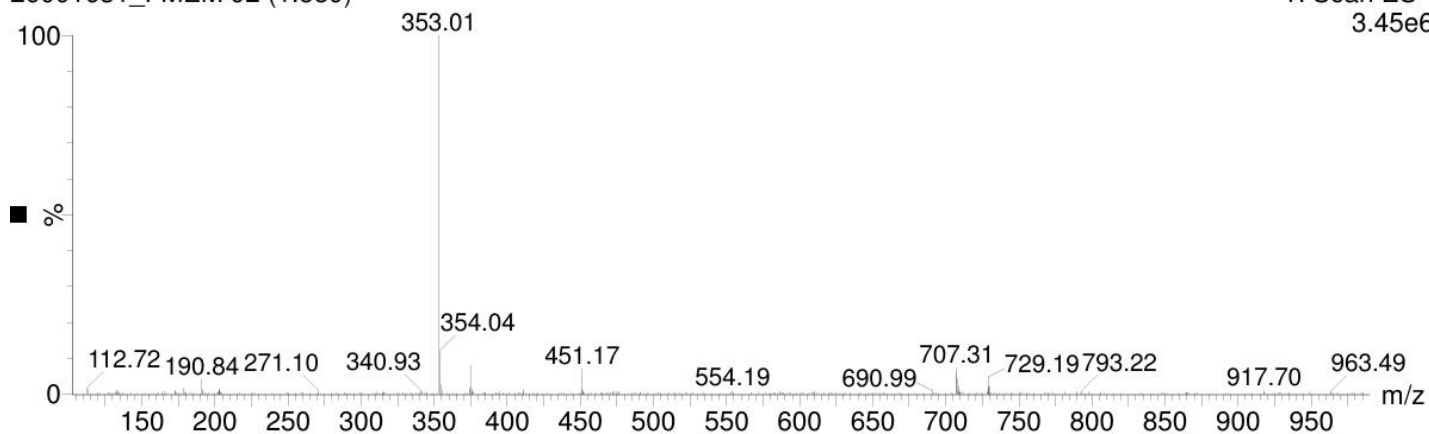
2: Scan ES+
7.80e6

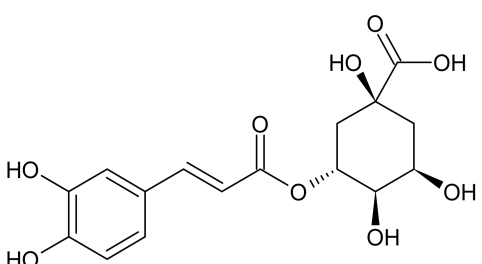


	Molecular weight	302
	Molecular ion peak	303
	Fragment	206

26001631_FMEM 92 (1.589)

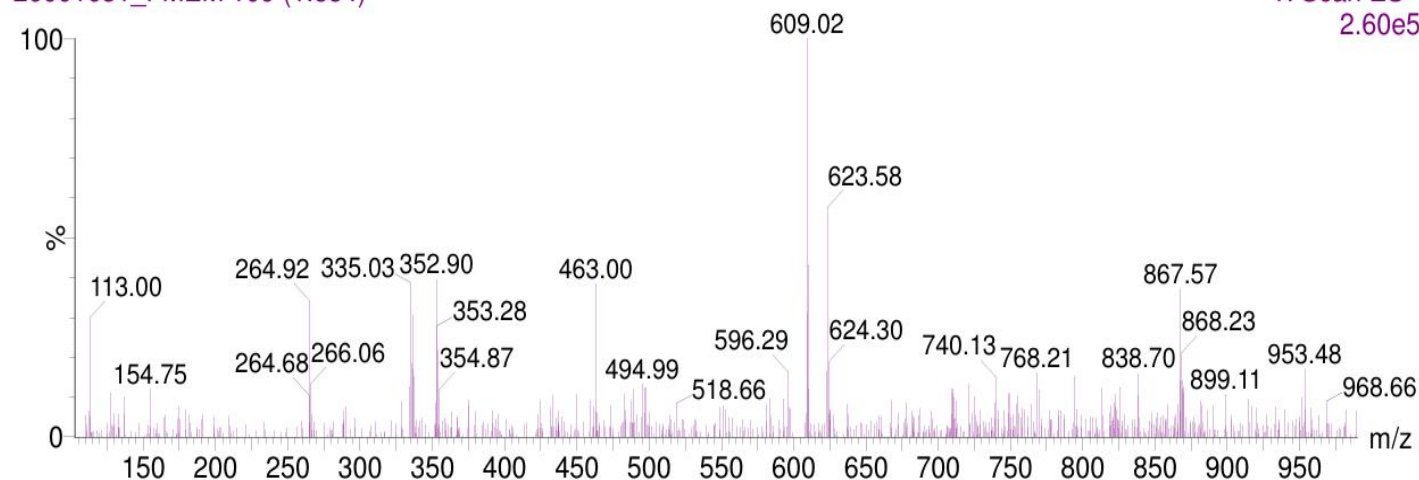
1: Scan ES-
3.45e6

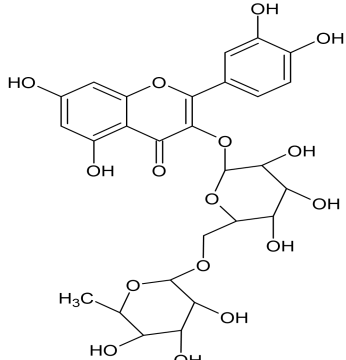


	Molecular weight	354
	Molecular ion peak	353
	Fragment	340

26001631_FMEM 109 (1.884)

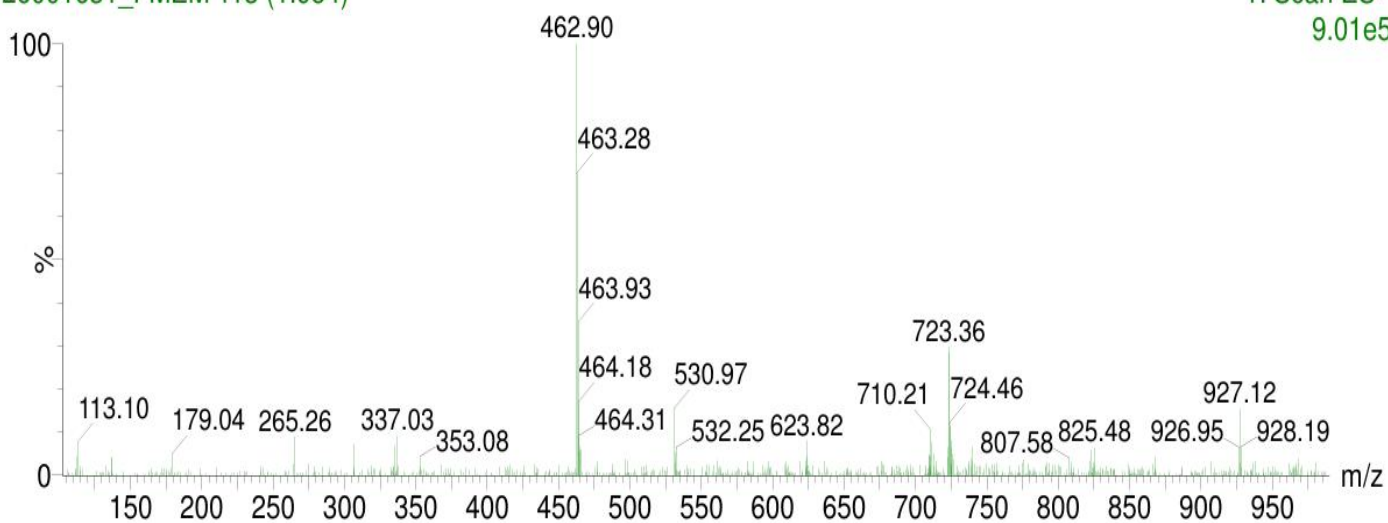
1: Scan ES-
2.60e5

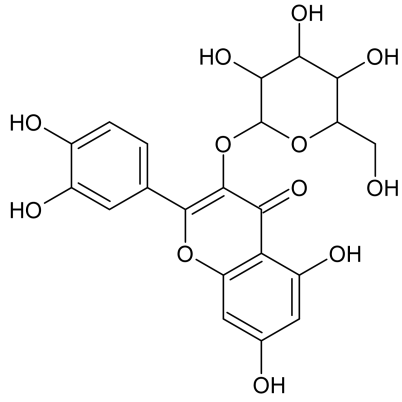


	Molecular weight	610
	Molecular ion peak	609
	Fragment	596

26001631_FMEM 113 (1.954)

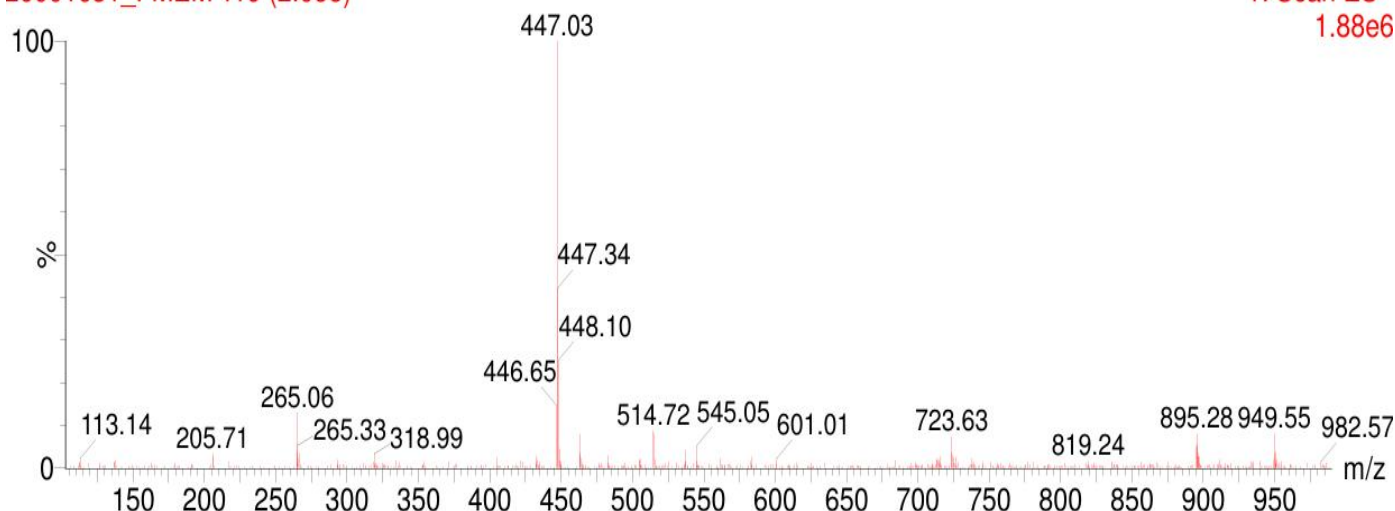
1: Scan ES-
9.01e5



	Molecular weight	463
	Molecular ion peak	462
	Fragment	353

26001631_FMEM 119 (2.058)

1: Scan ES-
1.88e6



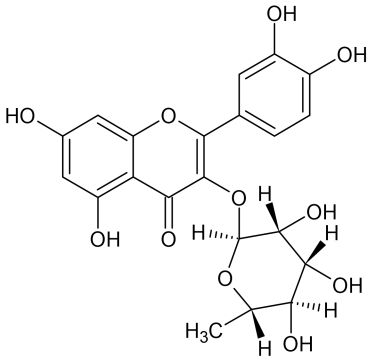
	Molecular weight	448
	Molecular ion peak	447
	Fragment	446

Table 5. Interpretation Data

Molecular Docking Study

Molecular docking was carried out for the selected phytoconstituents against three selected *Mycobacterium tuberculosis* protein targets (4QXM, 4NNH, and 5HJ7). The study included chlorogenic acid, m-tolyl dimethyl acetaldehyde, rutin, hyperoside, houttuynoside, quercetin, and quercitrin, along with the reference drugs isoniazid, pyrazinamide, and rifampicin. The analysis indicated favorable ligand–target interactions for several of the investigated phytoconstituents across the selected protein targets. The observed interactions provide preliminary evidence for the potential target-binding ability of these compounds and warrant further experimental investigation.

In Vitro Anti-tubercular Activity

The anti-tubercular activity of the methanolic extract of *H. cordata* (FMEM) was evaluated against *M. tuberculosis* H37Rv using the Microplate Alamar Blue Assay (MABA). The extract was tested over a concentration range of **100–0.2 µg/mL**, with rifampicin, isoniazid, and pyrazinamide used as reference drugs.

In the MABA, development of a **red colour** indicates mycobacterial growth, whereas retention of the **blue colour** indicates absence of detectable growth. The last well retaining the blue colour was considered the MIC endpoint.

The methanolic extract showed susceptibility at **100 µg/mL**, whereas no detectable inhibition was observed at the lower tested concentrations. Accordingly, the **minimum inhibitory concentration (MIC) of FMEM was determined as 100 µg/mL**.

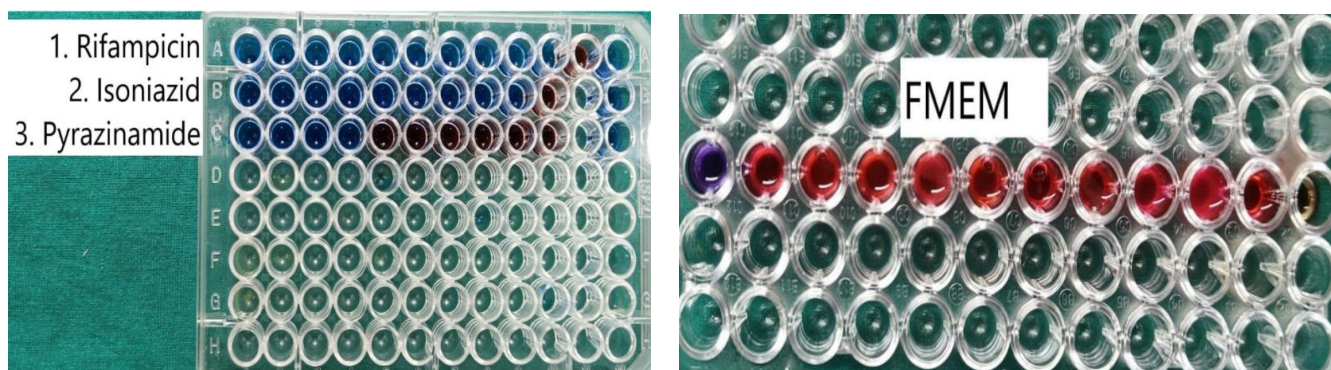


Figure 2: MABA Assay

CONCENTRATION	RIFAMPICIN	ISONIAZID	PYRAZINAMIDE	EXTRACT
100µg/ml	S	S	S	S
50µg/ml	S	S	S	R
25µg/ml	S	S	S	R
12.5µg/ml	S	S	S	R
6.25µg/ml	S	S	R	R
3.12µg/ml	S	S	R	R
1.6µg/ml	S	S	R	R
0.8µg/ml	S	S	R	R
0.4µg/ml	S	S	R	R
0.2µg/ml	S	R	R	R
POSITIVE CONTROL	G+	G +	G +	G +
DRUG CONTROL	NG	NG	NG	NG

Table 6. In vitro anti-tubercular activity of *Houttuynia cordata* extract

Overall Discussion

The study demonstrated that *H. cordata* contains several classes of phytoconstituents, including flavonoids and phenolic compounds, with the methanolic extract providing the highest reported extraction yield (16.30%). Spectroscopic and chromatographic analyses further supported the presence of diverse chemical constituents. Computational analysis showed favorable docking scores for several constituents, particularly rutin, houttynoside, and quercetin, against the selected *M. tuberculosis* targets. Importantly, the methanolic extract demonstrated *in vitro* anti-tubercular activity against *M. tuberculosis* H37Rv, with an observed MIC of 100 µg/mL. Taken together, the phytochemical findings, molecular docking results, and MABA outcome provide preliminary evidence supporting further investigation of *H. cordata* and its bioactive constituents as potential sources of anti-tubercular lead compounds. However, the docking findings are predictive and require confirmation through further biochemical, microbiological, and experimental studies.

IV. CONCLUSION

The present study demonstrated the preliminary anti-tubercular potential of *Houttuynia cordata* through phytochemical investigation, analytical characterization, molecular docking and *in vitro* evaluation. The methanolic extract (FMEM) showed susceptibility against *Mycobacterium tuberculosis* H37Rv at 100 µg/mL, with an MIC of 100 µg/mL, while lower concentrations showed resistance. Molecular docking revealed favorable interactions of selected phytoconstituents with relevant *Mycobacterium tuberculosis* protein targets, supporting their possible role in the observed activity. Overall, *Houttuynia cordata* may serve as a potential source of anti-tubercular bioactive compounds.

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