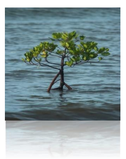
Profiling of Antibacterial Compounds from Selective Medicinal Mangrove Species



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Abstract

Mangrove is an opulent and untapped ecosystem with great phytochemical diversity, making it suitable for the discovery of novel antimicrobial compounds. The goal of the study was to explore the pharmaceutical antibacterial and antioxidant resources from *Bruguiera gymnorrhiza, Ceriops tagal, Rhizophora mucronata, and Aegiceras corniculatum* and gain insight into the diversity and novelty of compounds like alkaloids, flavanol, polyphenols, etc. A liquid extract was obtained by subjecting fresh mangrove leaves to Maceration & Soxhlet extraction. Plant DNA barcoding was utilized to authenticate the identity of the samples under study. A few of the obtained sequences have been communicated to GenBank (under review; accession number awaited). The phytochemical profiling revealed the presence of polyphenols (TPC = 8.71, 8.51, 8.77, 5.52 mg/gm of plant tissue resp.); flavonoids (TFC = 12.42, 8.48, 5.26, 13.903 mg/gm of plant tissue resp.); and alkaloids (2.5, 3.81, 4.98, 5.21 mg/gm of plant tissue resp.). The antioxidant potential (radical scavenging activity) was scored to be 87.8%, 89.5%, 92.07%, and 45.8% (DPPH assay was conducted). The antimicrobial analysis was performed on Staphylococcus aureus, *Escherichia coli, Klebsiella pneumoniae, and Bacillus subtilis*. The MIC revealed maximum activity in Klebsiella pneumonia, while negligible activity was scored for Staphylococcus aureus and Escherichia coli. The analysis thus reveals that the plants under study may have better medicinal activity against respiratory tract organisms. In-vitro Biochemical analysis of different molecules present in the plants was done using the Swiss ADME database. The present study thus reveals the preliminary compounds from selected mangrove plants that can be promising future anti-microbial therapeutics.

Aim and objectives:

The aim of the present study is to evaluate the antimicrobial properties of *Bruguiera gymnorrhiza, Ceriops tagal, Rhizophora mucronata, and Aegiceras corniculatum*

The objectives of the study were identified as;

- Genome based identification of plant samples collected Mumbai Mangrove reserved land (India)
- Screening of bioactive compounds present
- Study of antimicrobial activity on *Escherichia coli, Klebsiella pneumoniae, and Bacillus subtilis*

Methodology

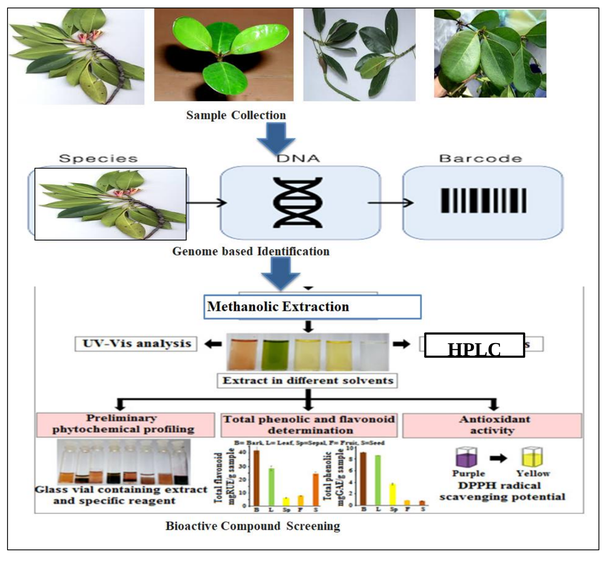

Fig 1.0 Phase I: Bioactive Compound Screening and Quantification

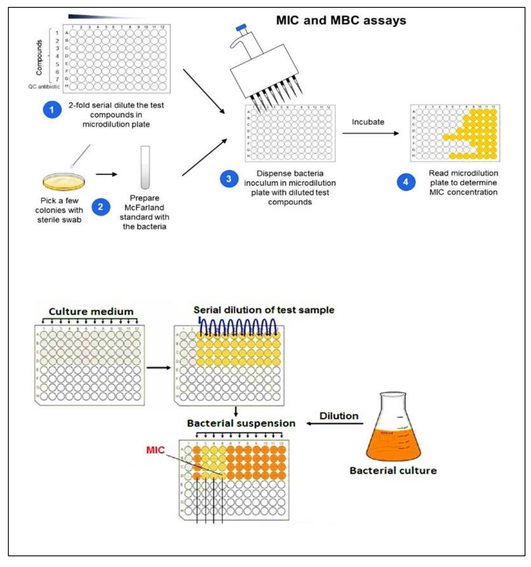

Fig 2.0: Phase II: Anti-microbial Screening (MIC)

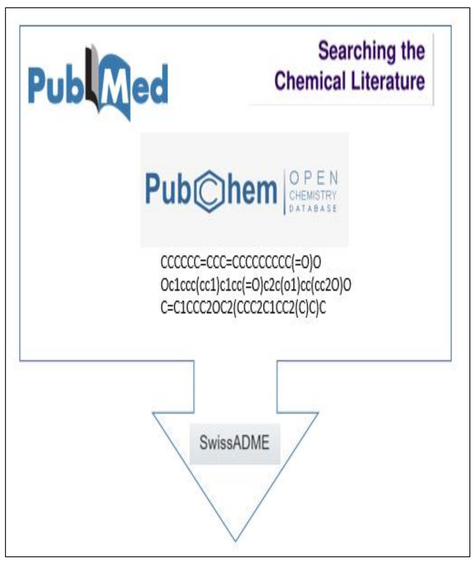

Fig 3.0 Phase III: In-silico ADME analysis

Results:

Determination of Flavonoids Content (TFC)

The total flavonoids content of four mangrove samples in their crude and 1:10 diluted forms was calculated and found to be -0.57115, -1.24231, -0.53846, 0.848075, -1.33846, -0.52692, 2.10565, and 13.9038 GAE/wet weight (gallic acid equivalent) for crude (A), 1:10 (A), crude (B), 1:10 (B), crude (C), 1:10 (C), and crude (110), respectively.

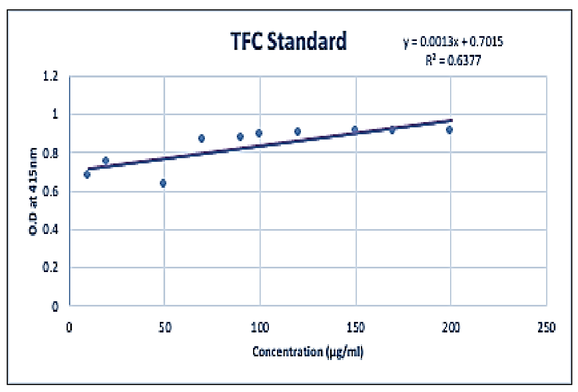

Fig 4.0: Quantitative estimation of TFC

Estimation of Total Phenolic Content (TPC)

Total phenolic content of four mangrove samples in their crude and 1:10 diluted forms was calculated and found to be 00.07274, 0.87119, 0.83833, 0.851305, 0.8625,0.8625 0.87785, 0.536425, and 0.5525 GAE/wet weight (Gallic acid equivalent) for crude (A), 1:10 (A), 1:10(A), Crude (B), 1:10 (B), Crude (C), 1:10 (C), Crude(D), 1:10(D).

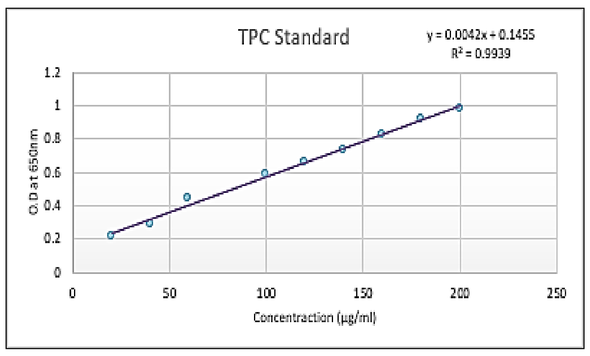

Fig 5.0: Quantitative estimation of TPC

DPPH (1,1-diphenyl-2-picryl hydrazine) Free Radical Scavenging (FRS) Assay

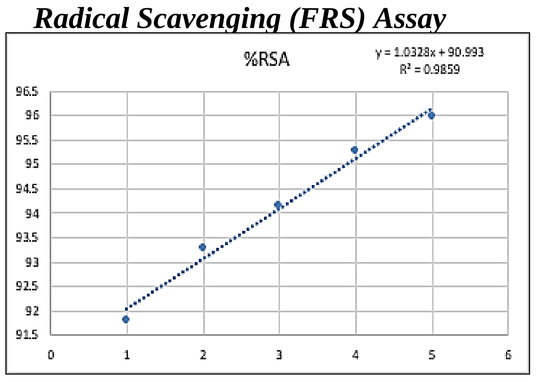

Fig 6.0: Anti-oxidant activity

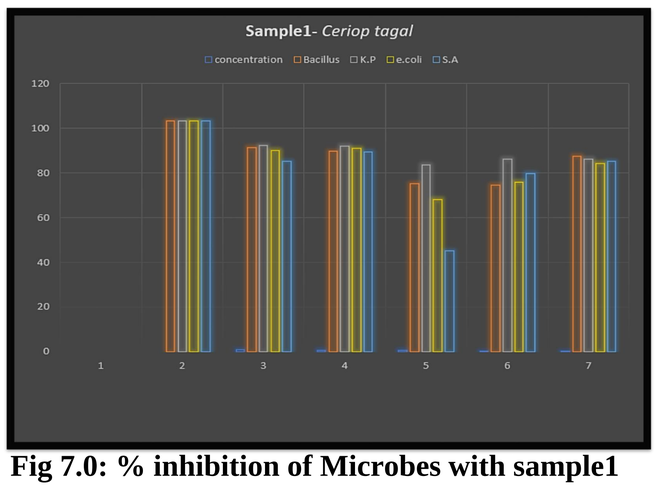

Fig 7.0: % inhibition of Microbes with sample1

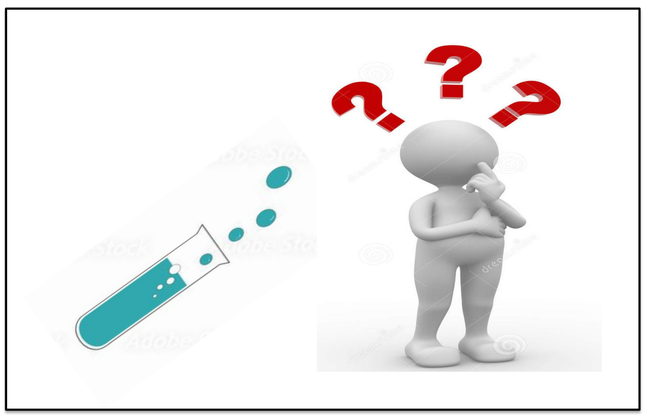

Fig 9.0: No significant result with sample 3

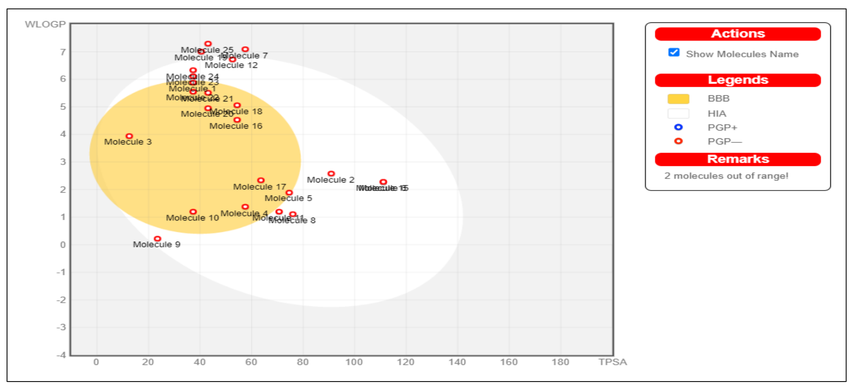

Fig 11.0: SWISSADME Boiled Egg analysis

Table 1: SWISSADME data, yellow colour highlighted are optimum

Molecule	Formula	ESOL Class	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	#violations	Lipinski #violation Score	Bioavailability Score	PAINS #alerts	Brenk #alerts	Synthetic Accessibility
Molecule 4	C9H8O3	Soluble	High	Yes	No	No	No	No	No	No	0	0.85	0.85	0	1	1.61
Molecule 5	C9H16O4	Very soluble	High	Yes	No	No	No	No	No	No	0	0.85	0	0	0	1.57
Molecule 10	C7H6O2	Very soluble	High	Yes	No	No	No	No	No	No	0	0.55	0	0	1	1
Molecule 17	C12H14O4	Soluble	High	Yes	No	No	No	No	No	No	0	0.85	0	0	0	1.99
Molecule 3	C15H24O	Soluble	High	Yes	No	No	Yes	Yes	No	No	0	0.55	0	0	2	4.35
Molecule 20	C16H33NO	Moderately soluble	High	Yes	No	Yes	No	No	No	No	0	0.55	0	0	0	2.12
Molecule 1	C18H32O2	Moderately soluble	High	Yes	No	Yes	No	Yes	No	No	1	0.85	0	0	1	3.1
Molecule 21	C18H35NO	Moderately soluble	High	Yes	No	Yes	No	Yes	No	No	1	0.55	0	0	1	2.97
Molecule 22	C16H32O2	Moderately soluble	High	Yes	No	Yes	No	Yes	No	No	1	0.85	0	0	0	2.31
Molecule 18	C18H30O3	Moderately soluble	High	Yes	No	Yes	No	Yes	Yes	No	0	0.85	0	0	2	3.44
Molecule 16	C18H28O3	Soluble	High	Yes	No	Yes	Yes	Yes	Yes	No	0	0.85	0	0	1	4.2
Molecule 8	C9H10O5	Very soluble	High	No	No	No	No	No	No	No	0	0.56	0	0	0	1.7
Molecule 9	C8H15NO	Very soluble	High	No	No	No	No	No	No	No	0	0.55	0	0	0	3.05
Molecule 12	C24H38O4	Poorly soluble	High	No	No	No	No	No	No	Yes	1	0.55	0	0	1	3.41
Molecule 11	C9H6O4	Soluble	High	No	No	Yes	No	No	No	No	0	0.55	1	0	2	2.61
Molecule 24	C18H36O2	Moderately soluble	High	No	No	Yes	No	No	No	No	1	0.85	0	0	0	2.54
Molecule 2	C15H10O5	Soluble	High	No	No	Yes	No	No	Yes	Yes	0	0.55	0	0	0	2.96
Molecule 6	C15H10O6	Soluble	High	No	No	Yes	No	No	Yes	Yes	0	0.55	0	0	0	3.14
Molecule 15	C15H10O6	Soluble	High	No	No	Yes	No	No	Yes	Yes	0	0.55	1	1	1	3.02
Molecule 23	C18H34O2	Moderately soluble	High	No	No	Yes	No	Yes	No	No	1	0.85	0	1	1	3.07
Molecule 7	C30H48O3	Poorly soluble	Low	No	No	No	No	No	No	No	1	0.85	0	1	1	6.21
Molecule 13	C21H20O11	Soluble	Low	No	No	No	No	No	No	No	2	0.17	1	1	1	5.04
Molecule 14	C21H20O11	Soluble	Low	No	No	No	No	No	No	No	2	0.17	1	1	1	5.17
Molecule 19	C30H50O2	Poorly soluble	Low	No	No	No	No	No	No	No	1	0.55	0	1	1	5.68
Molecule 25	C22H45NO	Poorly soluble	Low	No	No	Yes	No	No	No	No	1	0.55	0	0	0	2.82

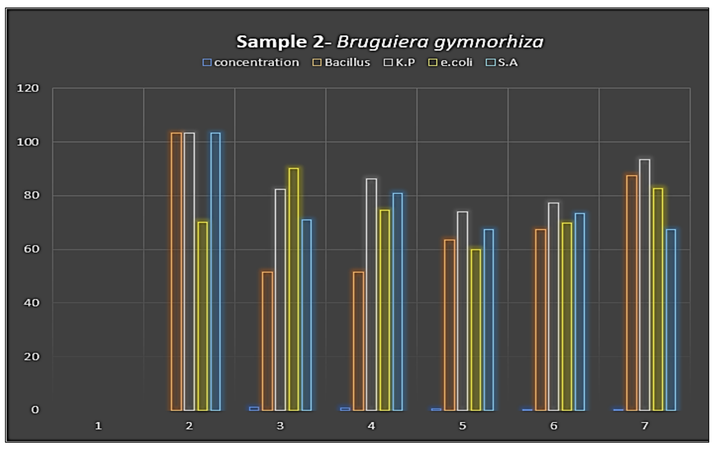

Fig 8.0: % inhibition of Microbes with sample 2

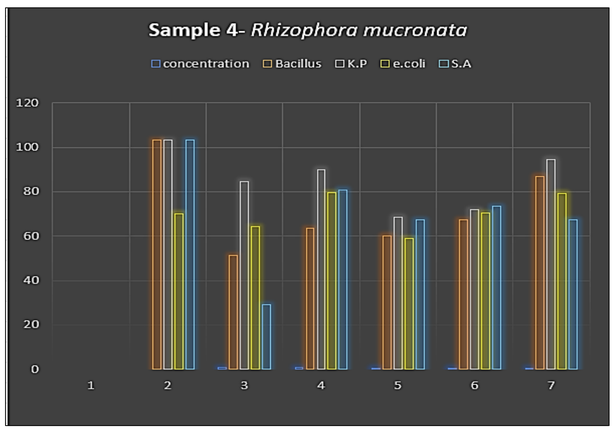

Fig 10.0: % inhibition of Microbes with sample4

Conclusion:

- Preliminary screening of the four species under study revealed a high amount of alkaloids, flavonoids, polyphenols, tannins and total proteins
- On the basis of barcode genes (matK, rbcl, ITS) genomic identification of species done (under communication with NCBI)
- Substantial amount of microbial inhibition was scored for *klebsiella* species and a moderate activity was recorded against *E.coli* and *Bacillus substillus*
- the plants under study may have better medicinal activity against respiratory tract organisms

Reference:

Antimicrobial activity of mangrove plant (Lumnitzera littorea). Asian Pac. J. Trop. Biomed., 4 (2011), pp. 523-525.

Database Resources of the National Center for Biotechnology Information. Nucleic Acids Res. 2022 Jan 7; 50(D1):D20-D26.

SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Sci. Rep. (2017) 7:42717.