IDENTIFICATION OF BRAHMA KAMAL METABOLITES AND ITS APPLICATION IN TARGETING EPIDERMAL GROWTH FACTOR RECEPTOR (EGFR) FOR TRIPLE NEGATIVE BREAST CANCER USING GC-MS/LC-MS AND IN SILICO TOOLS

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Phytochemical profiling, metabolites,GC-MS/LC-MS, EGFR, docking.

Introduction:

Triple Negative Breast Cancer (TNBC) is an aggressive subtype of breast cancer as it lacks these therapeutic targets, and does not respond to hormone therapy or HER2-directed drugs, making treatment difficult. TNBC cells frequently overexpress the Epidermal Growth Factor Receptor (EGFR), a key regulator of tumor growth, proliferation, and metastasis making EGFR an important molecular target for developing new therapeutic strategies. Medicinal plants have been a cornerstone of traditional and modern healthcare systems, serving as rich sources of bioactive compounds with therapeutic potential (Semwal *et al*., 2020). Traditionally, Brahma Kamal, has been widely used in Ayurvedic, Tibetan, and folk medicine systems for treating various ailment (Singh *et al.,* 2023). Different parts of the plant, are used for therapeutic purposes (Sharma *and* verma, 2025) because of presence of diverse phytochemicals such as flavonoids, phenolics, alkaloids, terpenoids, fatty acids, and glycosides (Semwal *et al*, 2025). These compounds are responsible for its wide range of pharmacological activities, including antioxidant, antimicrobial, anti-inflammatory, and wound-healing properties and cytotoxic acitivity. Advanced analytical techniques can identify metabolites which can be used for *in-silico* docking for triple negative breast cancer receptor targeting EPGR (Kaikade *et al*., 2023). Therefore, this project focuses on exploring the phytochemical composition and pharmacological potential of Brahma Kamala, and integrating it with molecular docking tools to identify the metabolite which can target triple negative breast cancer receptor (EGFR) and aims in natural drug development while promoting its conservation and scientific validation.

Objectives:

1. To collect and authenticate leaves of *Saussurea obvallata* plant material.
2. To prepare solvent extracts using leaves of plant and perform phytochemical analysis, GC-MS and LC-MS profiling to identify bioactive phytochemicals.
3. To screen the identified metabolites against the EGFR receptor associated with triple negative breast cancer (TNBC) using molecular docking and computational tools.

4. To evaluate the binding affinity, drug-likeness, and ADMET properties of the top bioactive Compounds.
5. To identify potential natural lead molecules with strong EGFR inhibitory potential for further anticancer drug development

Methodology:

A. Collection of samples
Leaves of Bramha kamala will be collected and authenticated by Taxonomist, P.C. Jabin Science College, Hubballi,

B. Sample preparation & extraction
Leaves of the plant will be collected and dried and solvents will be used for extraction of phytochemicals using Soxhlet extraction. The extract will be concentrated and used for analysis.

C. Chromatographic analysis
The phytochemical will be purified using chromatographic technique. It will be subjected to GC-MS and LC-MS analysis, which reveals the presence of secondary metabolites and its molecular weight.

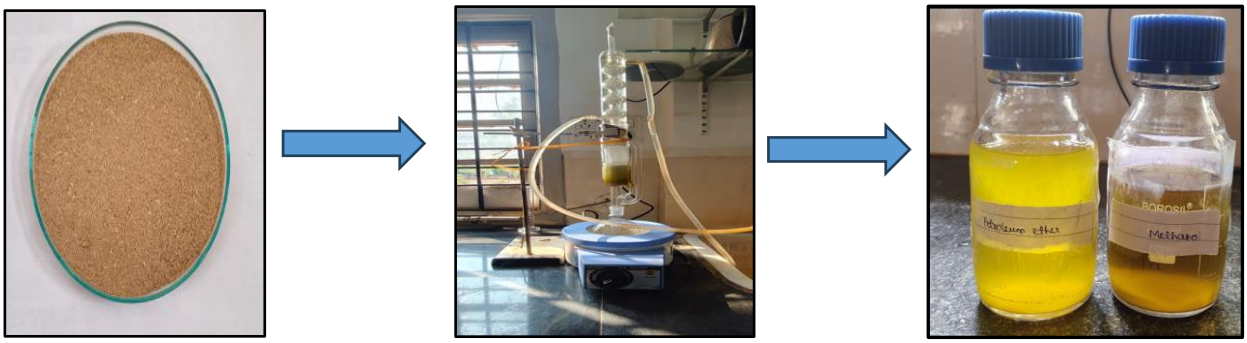
D. Compound selection & in silico ADMET
The target compounds will be selected using Lipinski rules and Swiss ADME and prioritize 5-8 highest-priority ligands.

E. Molecular docking
Targets: Proteins or receptors pertaining to particular disease like human EGFR 2 (Triple Negative Breast Cancer Receptor)
Tools: AutoDock Vina / PyRx for screening, followed by detailed interaction analysis in PyMOL / Discovery Studio. Record binding energies and interacting residues.

F. Identification of promising lead compounds targeting TNBCR.
Analysis of results and identification of lead compound having therapeutic potential.

Result and Conclusion:

The leaves of Brahma Kamala were collected and dired. The Phytochemicals were extracted using Soxhlet apparatus using solvents- methanol, petroleum ether (Figure 1). The phytochemicals were analysed using standard methods and results are recorded (Table 1 and Figure 2).



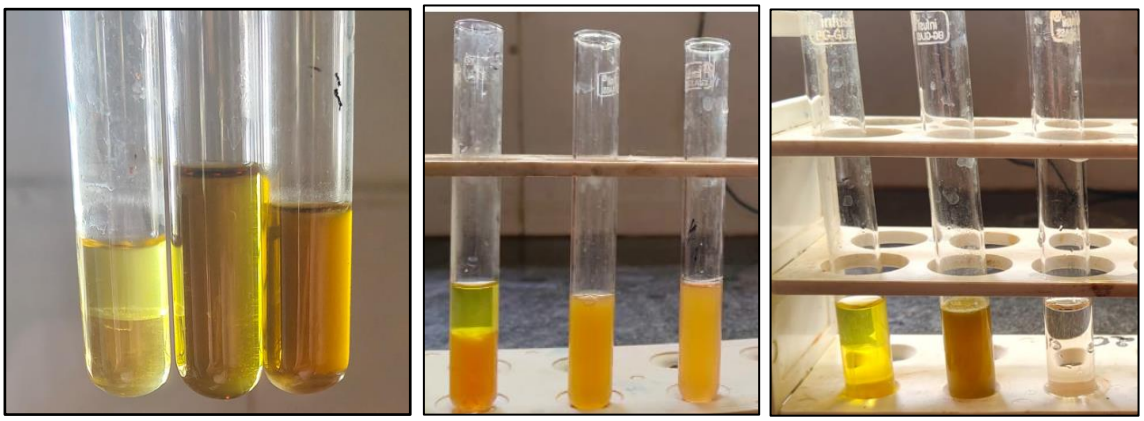
Powder of Brahma Kamala Leaves | Extraction using Soxhlet Apparatus | Extracted solvents

Figure 1: Extraction of phytochemicals using leaves

Table1: Phytochemical analysis of leaves of Brahma Kamala

Sl.No.	Metabolites	Test	*Methanol*	*Petroleum Ether*
01	Alkaloid Test	Mayer's Test	++	–
02	Flavonoids Test	Alkaline reagent Test	+	–
03	Glycosides Test	Keller-Kiliani Test	+	–
04	Phytosterol Test	Salkowski's Test	+	-
05	Carbohydrate Test	Fehling's Test	–	–
06	Tannin Test	Lead Acetate Test	+	–
07	Steroid Test	L-B Test	+	+
08	Terpenoid Test	Chloroform Test	+	+
09	Phenolic Test	Fecl3 Test	+	–
10	Saponin Test	Foam test	+	–
11	Protein and amino-acid Test	Ninhydrin test	–	–

The Methanolic extract revealed the presence of most of the metabolites compared to petroleum ether. The extracts are concentrated and the methanolic extract exhibiting more phytochemicals is submitted for metabolite analysis using GC-MS at SAIF, Karnataka University Dharwad. The result is awaited.



Test for Phenols Test for Terpenoids Test for Tanins

a) Petroleum ether extract b) methanol extract c) control

Figure 2: Phytochemical analysis of the extracts

Conclusion: The methanolic extracts showed the presence of metabolites compared to other solvent used for analysis. GC-MS analysis of the extract would reveal the presence of metabolites which will be identified using library. These metabolites will be used for *in-silico* studies.

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Future Scope:

1. Computational analysis: compound selection based on ADMET and Molecular docking studies.
2. Analysis for cytotoxic activity for Triple negative breast cancer cell lines.
3. Mechanism of action studies: Investigate pathways such as apoptosis, cell cycle arrest, and metastasis inhibition related to EGFR signalling.
4. In vivo studies: Conduct animal model studies to evaluate therapeutic efficacy, toxicity, and pharmacological effects.
5. Isolation and purification of compounds: Use chromatographic techniques to isolate active metabolites.
6. Structural characterization: Apply techniques like NMR and HR-MS for detailed identification of bioactive compounds.
7. Drug formulation development: Develop or formulate drug for targeting EGFR for triple negative breast cancer (TNBC).