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A COMPUTATIONAL FRAMEWORK FOR MODERN HERBAL DRUG DEVELOPMENT: "HERBAL DRUG MANUFACTURING: LAB - SMALL - LARGE SCALE INTEGRATED WITH ARTIFICIAL INTELLIGENCE"

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ABSTRACT

Herbal drug manufacturing is receiving increasing global interest because of the growing preference for natural, safe, and sustainable therapeutic goods. However, scaling up formulations from laboratory level to pilot and industrial production remains a significant challenge. Traditional scale-up methods mainly depend on trial-and-error approaches, which often lead to inconsistencies between batches, degradation or loss of active phytochemicals, lower extraction efficiency, excessive use of solvents and energy, and higher production costs. In addition, the lack of real-time monitoring and effective process control can negatively affect product quality and regulatory compliance. To overcome these challenges, the adoption of Artificial Intelligence (AI) along with advanced process analytical technologies has emerged as an effective solution. AI-driven systems are capable of predicting optimal extraction and processing conditions, reducing the need for repeated experiments, enabling real-time tracking of critical parameters, maintaining batch uniformity, improving yield, and optimizing resource usage. Furthermore, these technologies strengthen quality assurance and documentation processes. The integration of intelligent, data-driven approaches in herbal drug manufacturing not only increases efficiency but also supports sustainability and enhances global competitiveness. In the future, AI-powered smart manufacturing systems are expected to transform the herbal pharmaceutical industry by speeding up commercialization while ensuring safety, effectiveness, and regulatory compliance ***(Xiong, Hs. et al., 2023).***

KEYWORDS: Herbal drug manufacturing, Artificial intelligence, Process analytical technology (PAT), Phytoconstituent stability, Extraction optimization, Scale-up processing, Real-time monitoring, Quality assurance.

1. INTRODUCTION

Herbal medicinal products, derived from plant sources and their bioactive constituents form an essential component of traditional and modern healthcare systems worldwide. The manufacturing of herbal drugs begins at the laboratory level, where raw plant materials are collected, authenticated and subjected to initial extraction and formulation studies under controlled conditions. These preliminary stages involve selecting solvent systems, optimizing extraction parameters (e.g., maceration, decoction, percolation) and identifying active phytochemicals that confer therapeutic action. Extraction and formulation at this level aim to maximize the extraction of bioactive compounds while maintaining their chemical stability and structural integrity and activity - tasks that require careful analytical evaluation

of phytochemical profiles and bioactivity ***(Hardeep Singh, et al., 2023).***

Once promising formulations are developed at the lab bench the focus shifts toward small-scale pilot production, which serves as the critical link between laboratory concepts and large-volume manufacturing. Pilot-scale studies replicate the intended industrial processes in a controlled environment to optimize process parameters, evaluate reproducibility and validate production feasibility. This involves analyzing essential physical and chemical process factors, including heat and mass transfer. extraction kinetics and solvent usage. Systematic scale-up requires identifying key process parameters (CPPs) and essential quality attributes (CQAs) in yield, potency, and safety across batches. Pilot plants enable manufacturers to refine equipment selection, establish process flow designs, and resolve scale-specific issues such as variability in raw plant input and solvent behaviour — before committing to full production investments.

The final stage of the transition is large-scale or commercial manufacturing, where the optimized processes are implemented in full production units under stringent regulatory oversight. At this level, operations must comply with international good manufacturing practices (GMP) and quality standards to ensure that products consistently meet safety, efficacy and purity benchmarks. Large-scale manufacturing emphasizes batch uniformity, contamination control, equipment validation and documentation for traceability throughout the supply chain. It also incorporates robust quality control systems, such as chemical fingerprinting, marker-based quantification, and standardized analytical tests, to guard against adulteration and batch variability - concerns that become increasingly significant as production volume increases ***(Lamichhane, et al., 2023).***

A consistent challenge across all stages - from lab-scale extraction to industrial scale manufacturing - is maintaining the integrity and uniformity of bioactive phytochemicals despite the inherent variability of plant materials. Factors such as seasonal differences, geographic origin and plant part selection can influence the phytochemical profile, requiring adaptable process controls and validated analytical methods. Modern scale-up approaches engage formulation standardization, process analytical technology (PAT) and quality assurance systems that integrate traditional knowledge with scientific rigor. These measures help ensure that the transition from small experimental batches to large-scale production does not compromise therapeutic value while meeting regulatory and quality expectations (***Monika Shinde, et al., 2023).***

1.1. OVERVIEW OF HERBAL DRUG MANUFACTURING

Herbal drug manufacturing involves several steps to ensure quality, safety, and efficacy. It starts with selecting and authenticating medicinal plants, followed by processing steps such as cleaning, drying, size reduction, and extraction of bioactive phytochemicals. These are then formulated into suitable dosage forms and subjected to quality assurance ***(Averineni, RK. et al., 2024).***

1.2. NEED FOR LAB-TO-LARGE-SCALE TRANSLATION

Processes optimized at laboratory scale often fail during industrial scale-up due to changes in equipment design, heat and mass transfer, mixing efficiency and solvent behavior. Therefore, a systematic and scientifically guided scale-up approach is essential to ensure reproducibility and product quality (***Tchessalov S; Shalaev E; Bhatnagar B; et al., 2023).***

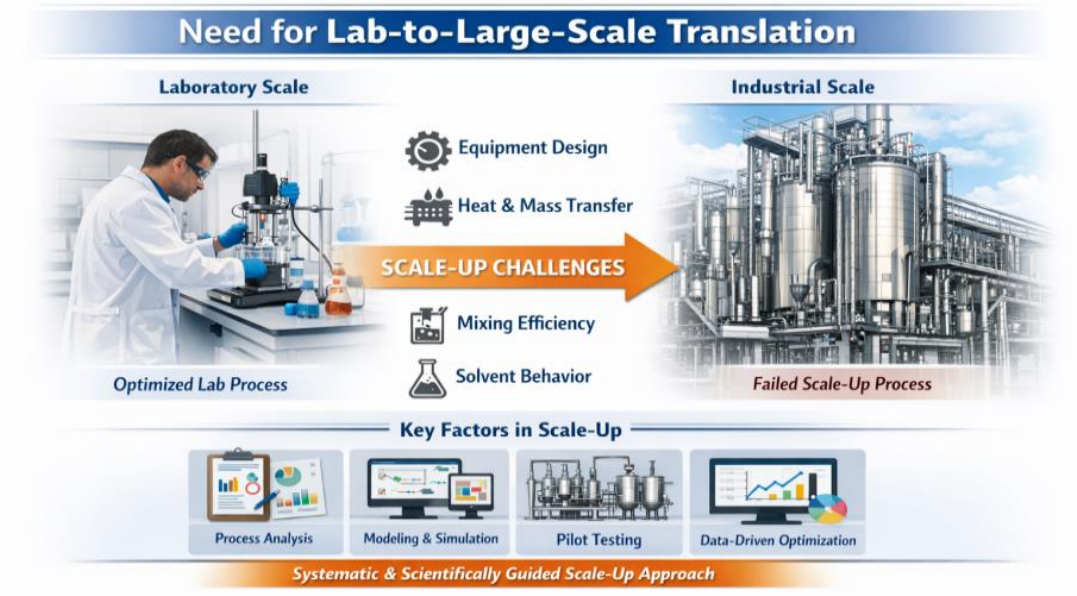

Figure 1: Need for lab-to-large scale Translation.

2. ROLE OF ARTIFICIAL INTELLIGENCE IN HERBAL DRUG MANUFACTURING

Natural products are compounds, substances, or mixtures derived from plants, animals, microbes, and other natural sources. For thousands of years, humans have relied on these products to treat various ailments, serving as the primary form of medicine before the development of modern pharmaceuticals. According to the World Health Organization (WHO), approximately 80% of the global population still uses traditional medicine today. Over the past five decades, natural products and their derivatives have continued to provide a valuable source of new drugs. However, large-scale utilization is often limited by challenges such as low bioavailability and complex chemical synthesis.

The rise of advanced computing, enhanced data storage, sophisticated natural language processing, and machine learning (ML) technologies now offers researchers powerful tools to study natural products more effectively. Artificial intelligence (AI) is enabling new possibilities in drug discovery, allowing medical science to harness nature's therapeutic potential more efficiently in the fight against human diseases.

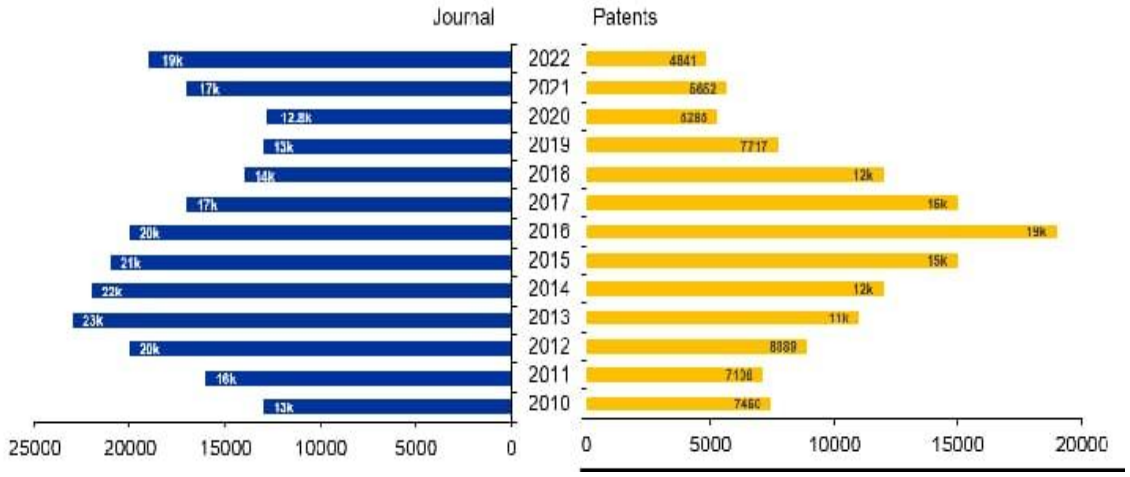

Figure 2: Number of journal and patent publications per year in natural product research (shown as blue and yellow bars, respectively) from 2010-2022 (Ralhan, K. et al., 2024).

Interest in applying AI to natural product research has grown rapidly in recent years, with around 650 journal and patent publications and a rising patent-to-journal ratio, reflecting increasing commercial interest. Although the total number of publications remains modest, there has been a consistent upward trend from 2010 to 2022, with a notable surge since 2020 (Figure 3). Analysis shows that China leads in publication output, followed by the U.S. and India. This dominance aligns with the widespread use of natural products in Chinese traditional medicine and China's implementation of the New Generation Artificial Intelligence Development Plan (2015–2030), which focuses on advancing AI-related capabilities nationally.

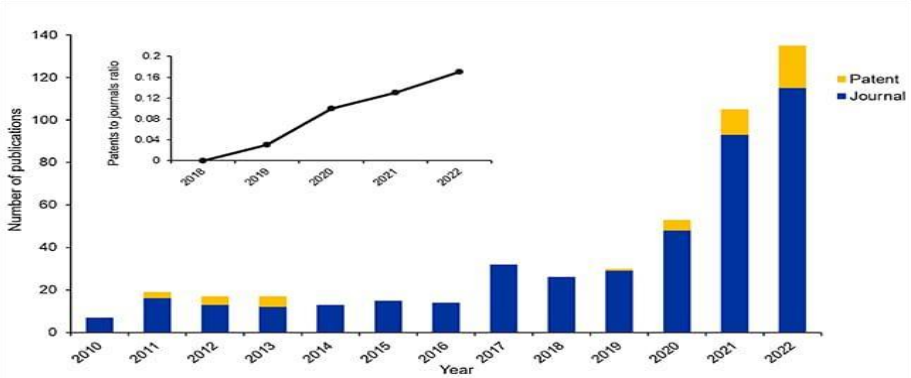

Figure 3: The annual number of journal and patent publications in the AI-driven natural product research field from 2010 to 2022, represented by blue and yellow bars, respectively. The inset illustrates the growth of the patent-to-journal ratio over the past five years (2018–2022), highlighting increasing commercial interest in this area (Ralhan, K. et al., 2024).

THE CURRENT LANDSCAPE OF AI AND NATURAL PRODUCTS

Currently, the most common AI application in natural product research is in developing anti-tumor agents (Figure 4A), followed by antiviral and antibacterial agents. Analgesics (pain-relieving drugs), although representing only a small portion (2%) of the top applications, experienced a fivefold increase in publications from 2021 to 2022 (Figure 4B). Other rapidly growing application areas include anti-inflammatory, anti-diabetic, anti-obesity, and antimalarial agents. Notably, the share of publications on antibacterial agents declined between 2021 and 2022, suggesting a reduced focus on this area within the scientific community ***(Ralhan, K. et al., 2024)***

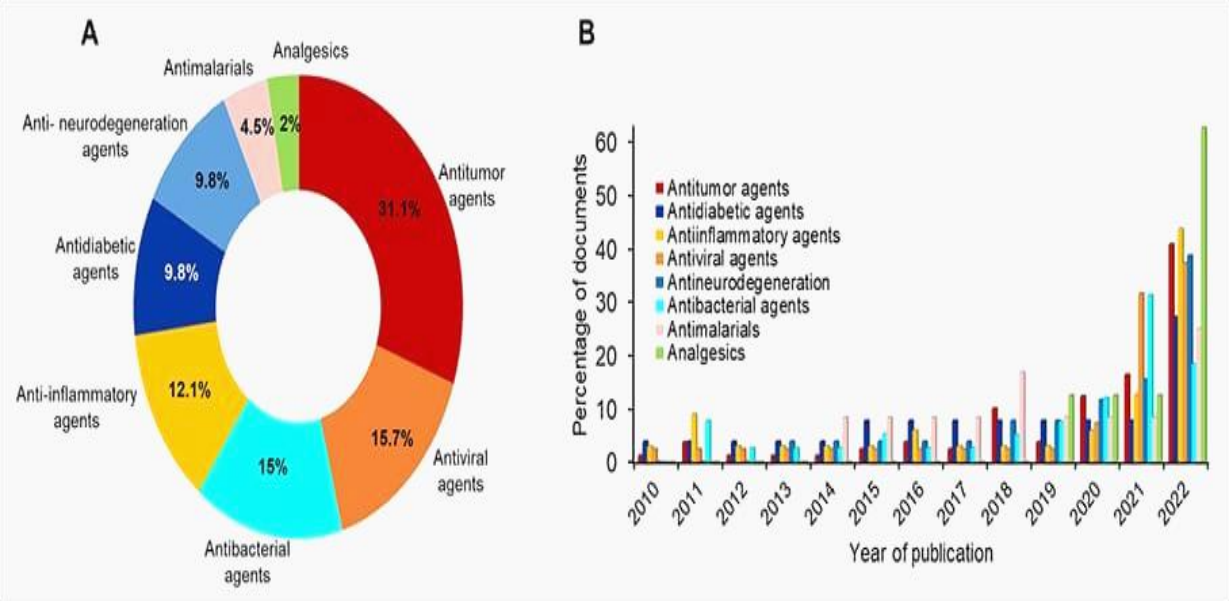

Figure 4: (A) Donut chart showing the leading applications of AI in natural product research. (B) Trend of AI adoption across the most frequently studied applications from 2010 to 2022. (Ralhan, K. et al., 2024)

2.1. WHY AI IS SUITABLE FOR COMPLEX HERBAL SYSTEMS

Herbal drugs are multicomponent, variable and biologically sensitive, which makes them very different from single-molecule synthetic drugs. AI fits naturally here because it thrives on complex, nonlinear systems.

1. Multicomponent Nature of Herbal Drugs

Herbal medicines are rich in phytochemicals, including alkaloids, flavonoids, terpenoids, and glycosides, which together contribute to their therapeutic effects. Unlike synthetic drugs, their activity often arises from synergistic interactions among multiple compounds rather than a single active ingredient. Artificial intelligence can process complex multivariate datasets to uncover relationships between phytochemical composition and biological activity, facilitating a deeper understanding of herbal drug efficacy.

2. High Variability in Raw Materials

The chemical composition of herbal raw materials can differ due to factors such as **geographical origin, climate, soil conditions, harvesting time, and storage practices**. Such variability can impact the consistency and quality of herbal formulations. AI systems can analyze both historical and real-time data to identify patterns in raw material variability and predict its effect on product quality, enabling manufacturers to adjust processing conditions and ensure batch-to-batch uniformity.

3. Non-Linear and Dynamic Processing Parameters

Herbal extraction and processing involve multiple interacting parameters such as **temperature, solvent ratio, extraction time, particle size, and pH**. These parameters often exhibit non-linear relationships that are difficult to model using traditional statistical approaches. AI techniques, including machine learning and neural networks, can capture these complex interactions and help optimize multiple parameters simultaneously, improving extraction efficiency and product quality.

4. Scale-Up Complexity (Lab to Industrial Scale)

During scale-up, variations in equipment design, mixing efficiency, and heat and mass transfer can cause **changes in yield, phytochemical composition, and overall**

product quality. AI-driven predictive models can use laboratory data to simulate process behavior at larger scales, allowing manufacturers to foresee potential challenges and optimize production conditions prior to full-scale industrial implementation.

5. Pattern Recognition and Quality Fingerprinting

Analytical techniques such as **HPLC, GC-MS, FTIR, and NIR spectroscopy** produce complex chemical fingerprints of herbal products. AI algorithms can rapidly analyze these spectral datasets to detect subtle variations, identify adulteration and ensure consistent chemical profiles between batches, thereby improving quality control.

6. Regulatory and Pharmacovigilance Support

AI supports regulatory compliance by enabling **continuous monitoring of manufacturing processes and automated quality documentation**. It can also analyze pharmacovigilance data to identify early safety signals and adverse reactions associated with herbal medicines, improving overall product safety and regulatory transparency (***Ankita Jaiswal, et al., 2025).***

3. LAB - SCALE MANUFACTURING OF HERBAL DRUGS

Lab-scale manufacturing is the initial and most critical stage in herbal drug development, where raw plant materials are converted into standardized herbal formulations under controlled conditions. At this scale, maintaining phytochemical consistency, quality and reproducibility is challenging due to the complex and variable nature of herbal materials.

Artificial Intelligence (AI) is crucial for optimizing every stage of lab-scale herbal drug manufacturing, providing data-driven insights, predictive capabilities, and enhanced process control.

3.1. OBJECTIVES OF LAB-SCALE MANUFACTURING

- ✧ To standardize extraction and formulation procedures.
- ✧ To optimize process parameters for maximum yield.
- ✧ To ensure quality, safety and reproducibility.
- ✧ To generate data for scale-up design and regulatory submission.

3.2. STEP-BY-STEP PROCESS

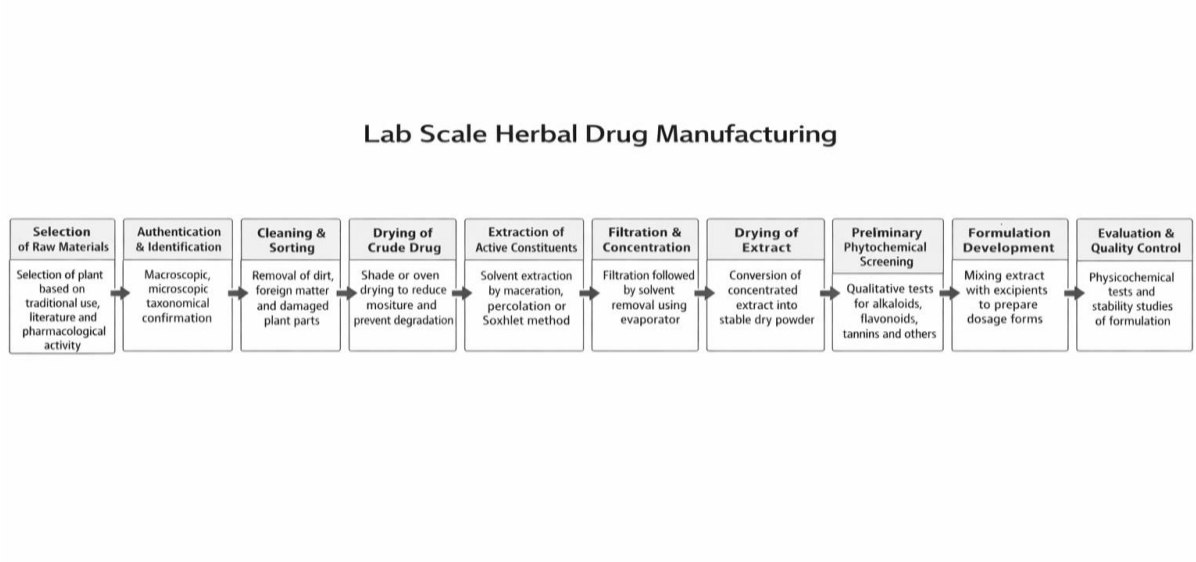

Figure 5: Step by step process of lab scale herbal drug manufacturing (Ahmad, I. et al., 2023).

4. SMALL SCALE MANUFACTURING OF HERBAL DRUG

Small-scale manufacturing of herbal drugs refers to the controlled production of herbal medicines in limited quantities for research, quality evaluation, optimization, or pilot-level distribution. Unlike large industrial batches, small-scale production emphasizes standardization, reproducibility and flexibility in processes. With rising demand for herbal products, researchers are integrating modern technology - especially Artificial Intelligence (AI) - to improve efficiency, quality and consistency (***Ke Z, et al., 2024).***

4.1. OBJECTIVES OF SMALL SCALE MANUFACTURING

- ➢ To standardize herbal drug production

Ensure batch-to-batch consistency in phytochemical composition.

- ➢ To optimize processing parameters

Identify ideal conditions for drying, extraction and formulation before large-scale production.

- ➢ To ensure quality, safety, and efficacy

Control microbial load, contaminants and active constituent levels.

➢ To reduce cost and material wastage
Use small quantities of raw material and solvents efficiently.

➢ To generate scientific and regulatory data
Produce reproducible data for scale-up, validation and regulatory submission.

➢ To integrate Artificial Intelligence (AI) tools
Improve prediction, monitoring and decision-making in herbal manufacturing processes.

4.2. STEP BY STEP PROCESS

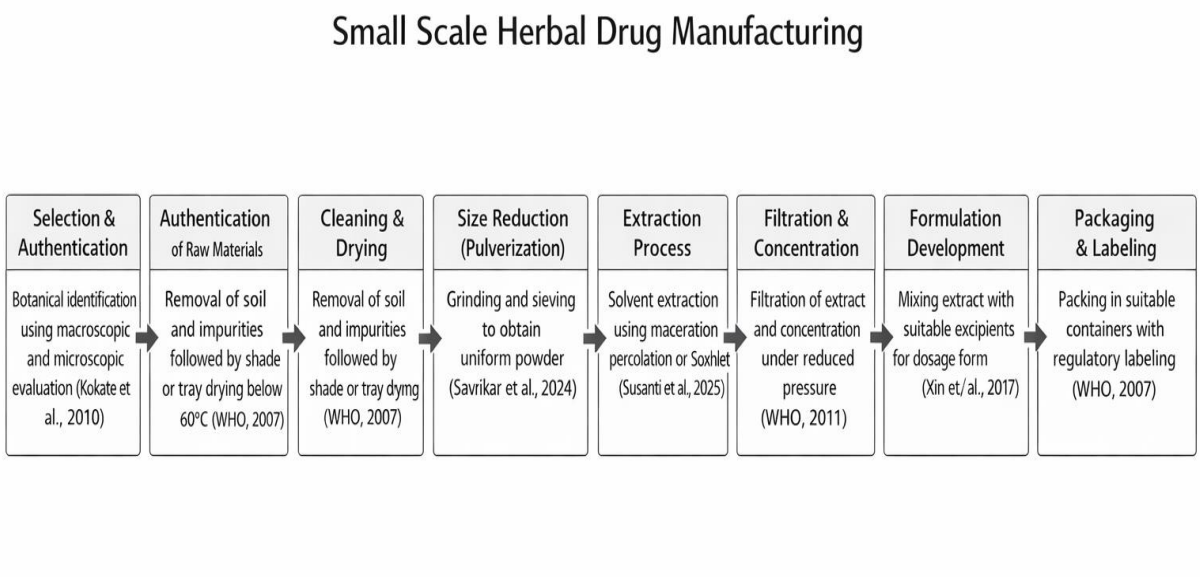

Figure 6: Step by step process of small scale herbal drug manufacturing.

4.3. DIFFERENCE BETWEEN LAB - SCALE AND SMALL-SCALE HERBAL DRUG MANUFACTURING

Laboratory-scale herbal drug manufacturing involves producing herbal formulations on a small scale under controlled conditions, primarily for experimentation, formulation development, or preliminary testing. It is usually performed in small quantities using laboratory equipment such as Soxhlet apparatus, rotary evaporator, mortar and pestle, hot air oven and analytical balance. The main objective of lab scale production is to standardize extraction methods, evaluate phytochemical constituents, determine stability, and optimize formulation parameters before commercial production. It focuses more on research, reproducibility and process validation rather than profit-oriented production. ***(Azmir, J. et al., 2013).***

Thus, the key difference lies in purpose, production quantity, equipment used, regulatory requirements and commercial intent. Lab scale focuses on research and development, whereas small-scale manufacturing focuses on limited commercial production with GMP compliance.

5. LARGE SCALE MANUFACTURING OF HERBAL DRUGS

The global demand for herbal medicines has increased significantly due to their therapeutic benefits and natural origin. Large-scale manufacturing is essential to meet market demand while maintaining stringent quality standards. However, herbal drugs pose unique challenges due to batch-to-batch variability, multi-component phytochemistry, and environment-dependent raw material quality. AI technologies provide advanced solutions to ensure consistency, optimize processes, and comply with regulatory requirements ***(Ralhan, K. et al., 2024).***

5.1. OBJECTIVES OF LARGE-SCALE HERBAL DRUG MANUFACTURING

- ✧ To produce uniform, high-quality herbal products at industrial scale
- ✧ To maintain batch-to-batch consistency of active constituents
- ✧ To comply with GMP and regulatory guidelines
- ✧ To reduce production cost, waste, and energy consumption
- ✧ To enable predictive process control and continuous improvement using AI

5.2. STEP BY STEP PROCESS

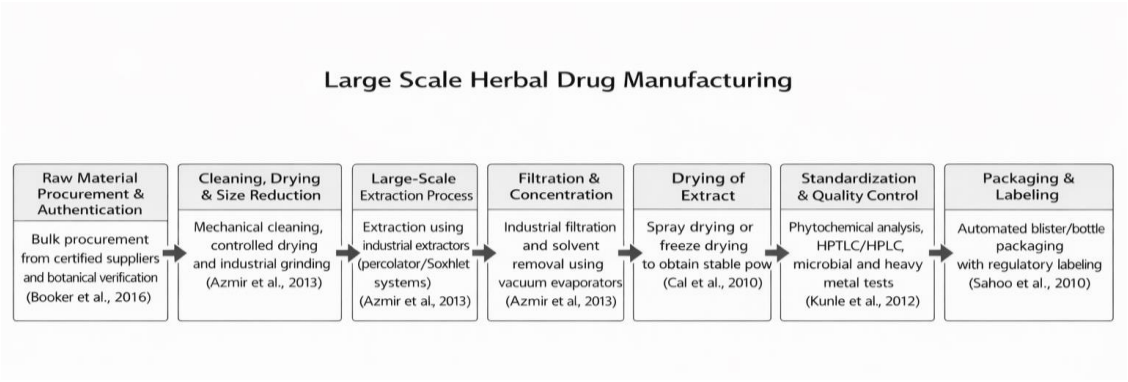

Figure 7: Step by step process of large scale herbal drug manufacturing.

5.3. DIFFERENCE BETWEEN SMALL-SCALE AND LARGE-SCALE HERBAL DRUG MANUFACTURING

Small-scale herbal drug manufacturing bear on limited batch production using semi-automatic or manual equipment with lower investment and simpler quality control facilities. It is mainly intended for local supply and traditional preparations, following basic GMP requirements. In contrast, large-scale manufacturing involves industrial-level production with high batch sizes, advanced automated machinery, sophisticated extraction and drying techniques, and strict regulatory compliance. Large-scale units maintain comprehensive quality control using advanced analytical methods to ensure uniformity, safety and international market standards ***(Sasidharan, S. et al., 2011).***

6. AI TOOLS INTEGRATED WITH LAB-SCALE TO LARGE-SCALE MANUFACTURING OF HERBAL DRUGS

Artificial Intelligence (AI) plays an important role in modern herbal drug manufacturing by improving accuracy and standardization from laboratory research to industrial production. In the lab stage, tools like PlantNet help in correct plant identification, while computational software such as AutoDock predicts the activity of phytochemicals. During small-scale production, platforms like MATLAB optimize extraction and processing conditions. In large-scale manufacturing, AI integrates with Process Analytical Technology (PAT) enables real-time monitoring and control of product quality during manufacturing. Thus, AI ensures better efficiency, safety and batch consistency in herbal drug production ***(Vig, et al., 2026; FDA, 2004).***

6.1. AI TOOLS

1. PLANT AUTHENTICATION(RAW DRUG IDENTIFICATION-LAB SCALE)

✓ **Pl@ntNet**

Pl@ntNet is an image-based plant identification app that can recognize various parts of a plant, including flowers, leaves, fruits, and bark. With extensive data collected over time, it is considered one of the largest mobile tools for plant identification ***(Goëau, Hervé, et al., 2013).***

Steps to Use Pl@ntNet

➢ **Install the App**

Download it from the Google Play Store or Apple App Store.

➢ **Open the App&Allow Location**

Launch Pl@ntNet to begin identifying plants and Enable GPS for better identification accuracy.

➢ **Tap "Identify"**

Take a clear photo of the plant (leaf, flower, fruit etc) or upload from gallery.

➢ **Select Plant Part**

Choose whether the image shows leaf, flower, fruit, bark etc.

➢ **Submit**

The app shows possible plant names with confidence scores.

➢ **Check & Confirm**

Compare images and select the correct species.

➢ **Save/Share (Optional)**

Save your observation or contribute to the community ***(Goëau; Hervé, et al., 2013).***

2. PHYTOCHEMICAL SCREENING AND PREDICTION (LAB SACLE)

✓ **DeepChem**

DeepChem is an open-source Python library for applying deep learning and machine learning methods to **molecular and chemical data** (such as small molecules, biochemical properties, ADMET prediction, bioactivity, etc.).

It does not inherently perform laboratory phytochemical extraction — instead it predicts molecular properties once data (such as structures or experimental labels) are available***(Vig Himangi et al., 2026).***

STEPS TO USE Deep Chem

✓ **Phytochemical Extraction(labwork)**

Extract plant material and identify compounds using GC-MS/HPLC.

➢ **Prepare dataset**

Collect SMILES structures of identified phytochemicals with activity/toxicity data.

➢ **Install DeepChem**

Set up phython environmental and install DeepChem.

➢ **Featurize molecules**

Convert SMILES into numerical features (e.g., graph fingerprints)

➢ **Train model**

Use models like GraphConvModel to train on activity data.

➢ **Evaluate Model**

Check accuracy (ROC-AUC, RMSE)

➢ **Predict & screen**

Predict activity/toxicity of new phytochemicals and rank promising candidates.

➢ **Experimental validatiom**

Validate top predicted compounds in laboratory assay ***(Vig Himangi et al., 2026).***

3. PROCESS OPTIMIZATION (SMALL SCALE MANUFACTURING)

✓ **Matlab**

MATLAB's AI capabilities, particularly through its Machine Learning Toolbox and Deep Learning Toolbox, can support herbal drug manufacturing by analyzing quality data, optimizing extraction and predicting bioactive compound profiles.

STEP-BY-STEP MATLAB PROCESS

➢ **Collect experimental data**

Prepare experimental samples of the herbal formulation with different component proportions.

Measure biological responses for each sample(e.g., activity or toxicity metrics)

➢ **Define Models variables**

Inputs: Concentration/dosage of herbal components

Outputs: Biological response values

➢ **Create ANN Model in MATLAB**

Use neutral network toolbox to build a back-propagation network.

➢ **Train the network**

train using experimental data until error is minimized.

➢ **Predict & optimize**

Run simulations with different component combinations and select the best predicted formulation.

➢ **Validate Experimentally**

Test the optimized formulation in lab experiments to confirm improvement (***Ren, Y.-S., et al., 2019).***

4. SCALE-UP MONITORING (LARGE SCALE MANUFACTURING)

✓ **Process Analytical Technology(PAT)**

The United States Food and Drug Administration (FDA) defines Process Analytical Technology (PAT) as a system for designing, analyzing, and controlling pharmaceutical manufacturing processes by measuring critical process parameters (CPPs) that influence the critical quality attributes (CQAs) of the product. For herbal and traditional medicine manufacturing, PAT has been adapted to enable **real-time monitoring and control of extraction, formulation, granulation and drying processes**, moving from a quality by testing approach to a quality by design paradigm.

STEPS TO USE PAT PROCESS

➢ **Define Critical Quality Attributes (CQAs)**

Identify key quality parameters such as active marker content, moisture, purity and stability.

➢ **Identify critical process parameters(CPPs)**

Determine variables affecting quality (temperature, pH, extraction time, solvent ratio etc.,)

➢ **Select suitable PAT tools**

Use real-time analytical techniques like NIR, Raman spectroscopy or mass spectroscopy.

➢ **Develop chemometric models**

Apply multivariate data analysis (PCA, PLS) to correlate analytical signals with quality attributes.

➢ **Implement Real-Time monitoring**

Install in-line/on line sensors during extraction, concentration or drying.

➢ **establish control strategy**

Use PAT feedback to adjust process parameters and maintain consistent quality.

➢ **validate during scale-up**

Confirm model accuracy when moving from lab scale to pilot scale.

➢ **Continuous Improvement**

Use collected data for optimization and process refinement ***(Xiong, HS. et al., 2023).***

5. QUALITY CONTROL & ADULTERATION DETECTION

AI-BASED SPECTRAL ANALYSIS SOFTWARE

✓ **SIRIUS**

SIRIUS is a bioinformatics software used to identify unknown metabolites from high-resolution tandem mass spectrometry (LC-MS/MS) uses both isotope patterns (MS^1) and fragmentation patterns (MS^2) to identify the molecular formula and predict the chemical structure of compounds in plant extracts. This helps in detecting

adulterants, contaminants and verifying phytochemical composition in herbal drugs (***Dührkop, K. et al., 2019).***

STEPS TO USE SIRIUS

- **Sample preparation**

Prepare herbal extract from plant material using suitable solvents.
Filter and inject the sample into **LC-HRMS/MS** for metabolomic analysis.

- **Acquire Mass Spectrometry Data**

Perform **LC-MS/MS analysis** to obtain high-resolution **MS^1 (isotope pattern)** and **MS^2 (fragmentation spectra)** of phytochemicals present in the herbal sample.

- **Convert Data Format**

Convert instrument files into compatible formats such as **.mzML or .mzXML** using tools like MSConvert.

- **Import Data into SIRIUS**

Open SIRIUS software and load the LC-MS/MS dataset.
The program automatically detects peaks and groups signals belonging to the same compound.

- **Set Instrument and Analysis Parameter**.

Define mass accuracy, ionization mode and possible adduct types.
Initialize algorithm parameters for isotope pattern extraction.

- **Molecular Formula Prediction**

SIRIUS calculates possible **molecular formulas** using isotope pattern decomposition and ranks them according to probability.

- **Fragmentation Tree Analysis**

The software reconstructs **fragmentation pathways** from MS/MS spectra to validate the predicted formula and structural fragments.

- **Structure Identification**

Using **CSI: FingerID**, predicted molecular fingerprints are searched in chemical databases (e.g., PubChem) to identify possible compounds.

- **Comparison with Authentic Herbal Profiles**

Identified metabolites are compared with reference phytochemical profiles of authentic herbal drugs.
Unexpected or foreign compounds indicate **possible adulteration or contamination**.

- **Quality Control Reporting**

Export results (PDF, XML, or text) showing identified metabolites, candidate structures and confidence scores for quality assessment.
These steps allow researchers to rapidly **screen herbal products, confirm authenticity and detect adulterated plant materials** using metabolomics-based analysis. ***(Böcker, S. et al., 2009).***

- ✓ **NIR Spectroscopy with AI-Based Chemometric Software**

Near-Infrared (NIR) spectroscopy with AI-based chemometric software is a rapid, non-destructive method used to analyze herbal drugs by measuring absorption of near-infrared light (780–2500 nm). The spectral data are processed using Machine Learning models, including PCA, PLS, and SVM, are used to identify phytochemical patterns, detect adulteration, and maintain quality control***(Li, X. et al., 2024).***

STEP TO USE NIR SPECTROSCOPY WITH AI-BASED CHEMOMETRIC SOFTWARE

- **Sample preparation**

Herbal materials (powder, leaves. or extract are collected and prepared in uniform form. The sample is placed in a suitable holder or sample cup for spectral analysis.

- **NIR Spectral Data Acquisition**

The prepared sample is scanned using an NIR spectrometer. The instrument records absorbance spectra produced by molecular vibrations of chemical bonds, including C–H, O–H, and N–H present in plant constituents.

- **Spectral Pre-processing**

The raw spectra are processed using chemometric software to remove noise and improve data quality. Techniques such as baseline correction, normalization, smoothing and derivative transformation are applied.

- **Chemometric Model Development**

Artificial intelligence -based chemometric models such as PCA, PLS-DA,SIMCA or SVM are developed using spectral data from authentic and adulterated herbal samples.

- **Pattern Recognition and Classification**

The AI model analyzes spectral patterns to differentiate genuine herbal samples from adulterated or contaminated ones by clustering and classification.

- **Quantification of Adulteration**

Regression models such as Partial Least Squares Regression(PLSR) estimate the level or percentage of adulterants present in the herbal material.

- **Validation of the Model**

The developed chemometric model is validated through external datasets or cross-validation to ensure its predictive accuracy and reliability.

- **Quality Control Decision**

The final prediction results are used in herbal drug manufacturing to confirm authenticity, detect adulteration, and ensure consistent product quality. NIR spectroscopy with chemometric modelling enables rapid, reagent free and It allows for non-destructive analysis, making it ideal for routine quality control of herbal medicines ***(Li, X. et al., 2024).***

DISCUSSION

From my perspective, the development of herbal drugs requires a well-structured transition from laboratory-scale research to small-scale and finally to large-scale industrial manufacturing ***(Balekundri, et al., 2020)***. At the laboratory level, the focus is mainly on selecting and authenticating plant materials, extracting bioactive compounds, and developing preliminary formulations ***(Heinrich, et al., 2018)***. However, processes that work efficiently in the laboratory often face difficulties during scale-up due to differences in equipment design, heat and mass transfer, and process control ***(Rathod, et al., 2019)***.

In my view, small-scale manufacturing plays a crucial role as it helps optimize processing parameters, evaluate reproducibility, and identify potential challenges before industrial production ***(Mukherjee, et al., 2019)***. This stage helps bridge the gap between experimental research and commercial manufacturing. Large-scale production then focuses on maintaining batch consistency, ensuring quality control and complying with regulatory standards such as GMP ***(Ram, et al., 2023)***.

I believe that the integration of Artificial Intelligence (AI) significantly improves herbal drug manufacturing by enabling predictive optimization, real-time monitoring and advanced quality control ***(Kumbhar, et al., 2024)***. AI-based analytical tools can analyze complex phytochemical data, detect adulteration, and ensure consistency in herbal formulations ***(Jaiswal, et al., 2024)***. Therefore, combining traditional herbal knowledge with modern AI technologies can enhance efficiency, product quality and global competitiveness in the herbal pharmaceutical industry ***(Paul, et al., 2021)***.

CONCLUSION

The development of herbal drugs requires a systematic progression from laboratory research to industrial-scale manufacturing. Laboratory studies establish the foundation through plant authentication, extraction and preliminary formulation, while small-scale production optimizes process parameters and ensures reproducibility. Large-scale manufacturing then focuses on maintaining batch consistency, quality control, and regulatory compliance such as Good Manufacturing Practices (GMP). The integration of Artificial Intelligence further strengthens this process by enabling predictive optimization, real-time monitoring and advanced analysis of phytochemical data. Overall, combining traditional herbal knowledge with modern AI technologies can significantly improve efficiency, quality and global competitiveness in herbal drug manufacturing.

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