

Advanced Pharmacognosy (Theory)

BP601T

A Textbook for B. Pharm. Semester VI

As per the new Pharmacy Council of India (PCI) Syllabus 2026 (NEP 2020)

Dr. Vishal Chauhan

Head of the department
(Pharmaceutical Chemistry)
Faculty of Pharmacy and Medical Science,
MAHSA University, Malaysia

Jyoti Pandit

Assistant Professor
School of Pharmaceutical Science, Jigyasa
University (Formerly Himgiri Zee
University), Uttarakhand, India

Manish Kumar

Assistant Professor
Department of Pharmacy,
Kingston Imperial Institute of Technology
& Science, Dehradun, India

Prof. Amol A. Ambekar

Assistant Professor
Godavari Shikshan Mandal's Asian
Institute of Pharmacy, Nashik,
Maharashtra, India



Advanced Pharmacognosy (Theory)

Course Code: BP601T

A Textbook for B.Pharm Semester VI

As per the new PCI Syllabus 2026 (NEP 2020)

Authors: Dr. Vishal Chauhan, Jyoti Pandit, Manish Kumar, Prof. Amol A. Ambekar

Edition: First Edition, August 2026

Language: English

Copyright © 2026 Wiseleaf Scientific Ventures Pvt. Ltd.

All rights reserved.

No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, recording, or otherwise, without the prior written permission of the publisher, except for brief quotations in reviews or scholarly works permitted by copyright law.

ISBN: 978-81-903393-9-1



MRP: 385/-

Published by: Wiseleaf Scientific Ventures Pvt. Ltd.

Address: Wework - Berger Delhi One Floor 19, C-001/A2, Sector 16b, Noida, Uttar Pradesh, 201301, India

Printed by: Patraloka | Prints and More

Immadihalli Main Rd, Immadihalli, Whitefield, Bengaluru, Karnataka 560066

Printed in India

Preface

Advanced Pharmacognosy occupies an unusual place in the pharmacy curriculum. It assumes a student who already knows crude drugs and phytochemistry, and it asks a harder question: how does a natural product become a validated, mechanistically understood, and legally protected medicine in the twenty-first century? The answer draws on disciplines that did not exist when classical pharmacognosy was written, from metabolomics and network pharmacology to artificial intelligence and access-and-benefit-sharing law, and it is these that the BP601T syllabus gathers under a single heading.

This book follows the syllabus unit by unit while telling one continuous story. It begins with reverse pharmacology and the traditional-knowledge record, the point at which a documented use becomes a research hypothesis. It proceeds through the analytical platforms that characterise a herbal drug as a metabolome, the computational and genomic methods that prioritise and explain its constituents, and the medicinal chemistry that turns an active constituent into an optimised lead. It ends with the preclinical, clinical, and regulatory evaluation that a lead must pass, and with the intellectual-property framework that protects both the innovation and the traditional knowledge it draws upon.

The treatment is pitched for the strong sixth-semester student and the examiner alike. Every unit opens on a concrete problem and supplies the tools to solve it; every technique is stated at the level of principle and then worked through with specific examples and, where the subject demands, with recomputed numerical problems. Original figures illustrate each method, and each chapter closes with a summary and a graded self-assessment that mirrors the university question pattern. Facts have been triangulated against standard references, and the book has been written to be accurate first and complete second.

The aim throughout is a book that serves three readers from the same pages: the first-time learner meeting metabolomics or network pharmacology for the first time, the reviser consolidating before the examination, and the researcher who will one day take a traditional claim into a modern laboratory.

Authors

Dr. Vishal Chauhan

Jyoti Pandit

Manish Kumar

Prof. Amol A. Ambekar

Course Objectives

The objectives of this course are to:

1. Understand reverse pharmacology and integrative approaches in natural drug discovery.
2. Apply metabolomics and systems biology tools for quality control and bioactivity evaluation of herbal medicines.
3. Explore modern AI-driven, in-silico, and high-throughput techniques for identification and optimization of natural product leads.
4. Study validation, safety, and development pathways of herbal leads including preclinical and clinical evaluation.
5. Understand legal, ethical, and patenting frameworks related to bioprospecting, traditional knowledge protection, and natural product innovation.

Course Outcomes

Upon successful completion of this course, the students will be able to:

1. Explain reverse pharmacology, traditional knowledge databases, and bioprospecting strategies.
2. Analyze herbal drugs using metabolomics, spectral libraries, and chemoinformatics tools.
3. Employ modern in-silico and AI techniques in lead identification and optimization from natural products.
4. Evaluate preclinical safety, pharmacokinetics, and efficacy of bioactive leads.
5. Interpret global IP frameworks and develop strategies for patenting herbal products and protecting traditional knowledge.

Syllabus

Unit	Topics	No. of lectures
I	Reverse Pharmacology and Integrative Approaches Reverse pharmacology and integrative approaches from the AYUSH perspective. Ethnopharmacological approach to bioprospecting. Traditional medicine databases: AYUSH Research Portal, ICMR Standards on Indian Medicinal Plants, TKDL, NAPRALERT, Super Natural, etc. Molecular docking and ADMET screening of bioactives. Concept of adjuvant therapy with herbals in metabolic and non-communicable diseases.	06 Hours
II	Metabolomics and Systems Biology Introduction to metabolomics and its tools: applications of NMR and HRMS in metabolomics, Metabolomics profiling and dereplication studies, Role of metabolomics in quality control, scientific validation of traditional claims and pharmacological evaluation, Network pharmacology and systems biology approaches to herbal medicine, Significance of spectral libraries and chemoinformatics databases in drug discovery.	11 Hours
III	Modern Techniques in Natural Product Discovery Role of artificial intelligence (AI), Machine learning and big data in Drug discovery from natural Products. Molecular docking, Virtual Screening and Pharmacophore modelling, Use of Genomic and transcriptomic tools in medicinal plant research, High-throughput screening (HTS) and bioautography.	10 Hours
IV	Validation and Development of Herbal Leads Bioactivity Guided Fractionation, characterization/Structure Elucidation, Optimization of lead compounds for better efficacy, safety, and stability through SAR and QSAR modelling for semi-synthetic compounds of Salicin, Artemisinin, Piperine, Papaverine and Andrographolides. Preclinical, Clinical Evaluation and New Drug approvals: Testing for toxicity as per OECD guidelines, pharmacokinetics, and bioavailability of herbal products, extracts and lead compounds, assessment of safety and efficacy, clinical trials with or without placebo for clinical endpoints based on assessment of quality of life reporting adverse events if any, filing IND application, NDA submission, Regulatory review and post marketing surveillance.	12 Hours
V	Patenting of Natural Products	06 Hours

	Key Terminologies and Concepts: Definitions and distinctions: Patent, Intellectual Property Rights (IPR) Farmers' Rights and Breeders' Rights, Bioprospecting and Biopiracy. Patenting Aspects of Natural Products and Traditional Knowledge: Legal frameworks and challenges in patenting natural substances, Traditional Knowledge Digital Library (TKDL) and its role in protecting indigenous knowledge. Role of National Biodiversity Authority in patenting natural products and NAGOYA protocol. Case Studies: Turmeric U.S. patent on wound healing and its revocation; Neem biopiracy issue and patent cancellation.	
--	--	--

Table of Contents

Preface.....	iii
Chapter 1. Reverse Pharmacology and Integrative Approaches.....	1
Learning outcomes	1
1.1 Introduction	1
1.2 Reverse pharmacology and the integrative AYUSH framework.....	2
1.3 The ethnopharmacological approach to bioprospecting.....	4
1.4 Traditional-medicine databases.....	6
1.5 Molecular docking and ADMET screening of bioactives.....	9
1.6 Adjuvant therapy with herbals in metabolic and non-communicable diseases.....	13
1.6A Ethnopharmacological field methodology and quantitative indices	15
1.6B Adjuvant mechanisms in metabolic disease, in more detail.....	16
Key revision points.....	17
1.7 Chapter summary	18
1.8 Self-assessment	18
1.9 References	23
Chapter 2. Metabolomics: Principles and Analytical Platforms.....	24
Learning outcomes	24
2.1 Introduction	24
2.2 The metabolome and the metabolomic workflow.....	25
2.3 Nuclear magnetic resonance spectroscopy in metabolomics	28
2.4 High-resolution mass spectrometry in metabolomics	30
2.5 Choosing a platform	34
2.6 Metabolomic profiling and data processing.....	35
2.6A Two-dimensional NMR experiments	37
2.6B Tandem mass spectrometry and quality assurance of a metabolomic run	38
Key revision points.....	38
2.7 Chapter summary	39
2.8 Self-assessment	40
2.9 References	44
Chapter 3. Dereplication, Network Pharmacology and Systems Biology	45
Learning outcomes	45
3.1 Introduction	45

3.2 Dereplication	46
3.3 Spectral libraries and chemoinformatics databases.....	49
3.4 Metabolomics in the quality control of herbal drugs	50
3.5 Scientific validation of traditional claims and pharmacological evaluation	51
3.6 Network pharmacology	52
3.7 Systems biology	55
3.6A Building a network-pharmacology model in practice	56
3.6B Molecular networking as a practical workflow	58
Key revision points.....	58
3.8 Chapter summary	59
3.9 Self-assessment	60
3.10 References	63
Chapter 4. Artificial Intelligence, Machine Learning and Big Data in Natural Product Discovery	65
Learning outcomes	65
4.1 Introduction	65
4.2 Artificial intelligence, machine learning, and deep learning	66
4.3 Types of machine learning	67
4.4 The machine-learning workflow in drug discovery	69
4.5 Big data in natural-product discovery	73
4.6 Applications and limitations.....	73
4.6A The principal algorithms, explained.....	75
4.6B Generative models and de novo design	76
Key revision points.....	76
4.7 Chapter summary	77
4.8 Self-assessment	78
4.9 References	81
Chapter 5. In-silico Screening, Genomics and High-Throughput Methods	82
Learning outcomes	82
5.1 Introduction	82
5.2 Molecular docking.....	83
5.3 Virtual screening	86
5.4 Pharmacophore modelling.....	88
5.5 Genomic and transcriptomic tools in medicinal-plant research	89

5.6 High-throughput screening.....	90
5.7 Bioautography	92
5.6A High-throughput screening formats and hit triage	93
5.6B Genome mining and silent gene clusters, in more detail	94
Key revision points.....	95
5.8 Chapter summary	95
5.9 Self-assessment	96
5.10 References	100
Chapter 6. Validation and Optimization of Herbal Leads: Bioactivity-Guided Fractionation, SAR and QSAR	101
Learning outcomes	101
6.1 Introduction	101
6.2 Bioactivity-guided fractionation	102
6.3 Characterization and structure elucidation	104
6.4 Optimisation of lead compounds.....	105
6.5 Structure-activity relationships (SAR).....	106
6.6 Quantitative structure-activity relationships (QSAR).....	107
6.7 The five leads as worked cases	110
6.6A Descriptors and three-dimensional QSAR	114
6.6B Biosynthesis and the supply of a natural lead.....	115
Key revision points.....	116
6.8 Chapter summary	116
6.9 Self-assessment	117
6.10 References	121
Chapter 7. Preclinical, Clinical Evaluation and Regulatory Approval	122
Learning outcomes	122
7.1 Introduction	122
7.2 Preclinical toxicity testing under OECD guidelines	124
7.3 Pharmacokinetics and bioavailability of herbal products	126
7.4 Assessment of safety and efficacy: clinical trials.....	129
7.5 New-drug approval and post-marketing surveillance	132
7.5A Compartmental pharmacokinetics and its parameters.....	132
7.5B Good practices and the Indian regulatory setting	134
Key revision points.....	134

7.6 Chapter summary	135
7.7 Self-assessment	136
7.8 References	140
Chapter 8. Patenting of Natural Products and Traditional Knowledge	141
Learning outcomes	141
8.1 Introduction	141
8.2 Key terminologies	142
8.3 Patenting natural products and traditional knowledge	144
8.4 The Traditional Knowledge Digital Library	146
8.5 The National Biodiversity Authority and the Nagoya Protocol.....	147
8.6 The turmeric and neem cases	148
8.6A The international system and the Indian Patents Act	150
8.6B Geographical indications and the wider protection of heritage.....	152
Key revision points.....	152
8.7 Chapter summary	153
8.8 Self-assessment	154
8.9 References	158