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PHARMACOGNOSY AND PHYTOCHEMISTRY - II

UNIT 2

TOPIC :

- **Phenylpropanoids and Flavonoids : Lignans, Tea, Ruta**



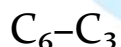
Phenylpropanoids and Flavonoids

- Phenylpropanoids and flavonoids are important groups of secondary metabolites produced by plants.
- They are derived mainly from the amino acid phenylalanine and play crucial roles in plant defense, pigmentation, growth regulation, and human health.

Phenylpropanoids

- Phenylpropanoids are a diverse class of organic compounds derived from the amino acid phenylalanine (and sometimes tyrosine).
- They are characterized by a phenyl ring (C_6H_5-) attached to a three-carbon side chain (C_3) — forming the basic structure C_6-C_3 .

General Structure



(Benzene ring + three-carbon side chain)

Biosynthetic Origin

→ Phenylpropanoids are formed through the shikimic acid pathway → phenylalanine → trans-cinnamic acid → other derivatives.

Examples

1. Cinnamic acid
2. Coumarins (e.g., umbelliferone, scopoletin)

Functions in Plants

- Provide structural support (e.g., lignin in cell walls)
- Act as UV protectants
- Serve as defense compounds against herbivores and pathogens

Pharmacological / Therapeutic Importance

- Antioxidant properties
- Anti-inflammatory effects
- Antimicrobial and antiviral activity

Examples of Drugs / Compounds

Compound	Source	Uses
Cinnamic acid	Cinnamon	Flavoring agent, antimicrobial
Coumarin	Tonka bean	Anticoagulant precursor
Eugenol	Clove oil	Analgesic, antiseptic

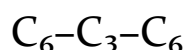
Flavonoids

- Flavonoids are a large group of polyphenolic compounds derived from phenylpropanoid and acetate pathways.
- They are characterized by a $C_6-C_3-C_6$ structure, consisting of two aromatic rings (A and B) connected by a three-carbon bridge forming a heterocyclic ring (C).

Basic Structure

- Two aromatic rings (A and B)
- Linked by a three-carbon chain, forming a heterocyclic ring (C)
- General formula: $C_{15}H_{10}O_2$

Skeleton:



Classification of Flavonoids

Based on oxidation and substitution pattern of the central C-ring:

Class	Example	Source	Remark
Flavones	Apigenin, Luteolin	Parsley, celery	Anti-inflammatory
Flavonols	Quercetin, Kaempferol	Onion, tea	Antioxidant
Flavanones	Naringenin, Hesperidin	Citrus fruits	Antioxidant
Flavanols (Catechins)	Epicatechin	Green tea, cocoa	Cardioprotective
Anthocyanidins	Cyanidin, Delphinidin	Berries, grapes	Pigments, antioxidant
Isoflavones	Genistein, Daidzein	Soybeans	Estrogenic activity

Biosynthesis

- Derived from phenylpropanoid pathway (from phenylalanine) and acetate pathway (malonyl-CoA).
- Involves chalcone synthase enzyme forming chalcone, which cyclizes into different flavonoids.

Functions in Plants

- Provide flower coloration (attract pollinators)
- Act as UV filters and antioxidants
- Involved in symbiotic nitrogen fixation
- Protect plants from pathogen attack

Pharmacological / Therapeutic Importance

- Antioxidant → prevents oxidative stress
- Anti-inflammatory → inhibits prostaglandin synthesis
- Anticancer → modulates carcinogen metabolism
- Cardioprotective → reduces LDL oxidation
- Hepatoprotective and neuroprotective
- Some flavonoids show antiviral and antibacterial activities

Lignans

- Lignans are a group of natural organic compounds found in many plants, especially in seeds, grains, vegetables, and fruits.
- They are phenolic compounds formed by the joining of two phenylpropanoid units (C₆–C₃ units).
- Lignans act as antioxidants and show estrogen-like and anticancer activities.
- They are considered secondary metabolites and play a role in plant defense against microorganisms.
- Common plant sources include flaxseed, sesame, whole grains, and legumes.

Composition

- Main Components: Phenolic compounds made from two C₆–C₃ units (phenylpropane units).
- Precursors: Derived from the amino acid phenylalanine through the shikimic acid pathway.
- Contain phenolic hydroxyl groups, which are responsible for antioxidant properties.
- Some important lignans include:
 - Secoisolariciresinol
 - Matairesinol
 - Podophyllotoxin
 - Enterolactone
 - Enterodiol



Chemistry and Chemical Classes

- Chemical Nature: Lignans are dimers of phenylpropanoid units linked by a C–C bond (usually at the β – β' position).
- Basic Skeleton: Two benzene rings each with a three-carbon side chain (C₆–C₃ units).
- Chemical Classes:
 1. Simple lignans – e.g., secoisolariciresinol
 2. Dibenzylbutane lignans – e.g., enterolactone
 3. Aryltetralin lignans – e.g., podophyllotoxin
 4. Furofuran lignans – e.g., sesamin

Biosources

- Natural Sources:
 - Flaxseed (*Linum usitatissimum*) – richest source of secoisolariciresinol
 - Sesame seeds (*Sesamum indicum*) – contains sesamin and sesamolin
 - Podophyllum species – contains podophyllotoxin
- Plant Parts Used: Seeds, roots, and bark.
- Formation in Plants: Produced through the phenylpropanoid pathway, mainly from phenylalanine.

Therapeutic Uses

Lignans show many biological and medicinal effects:

Compound	Therapeutic Use
Podophyllotoxin	Used in preparation of anticancer drugs like <i>etoposide</i> and <i>teniposide</i>
Secoisolariciresinol	Antioxidant, cardioprotective, and hormone-balancing effects
Sesamin	Lowers cholesterol and has liver-protective activity
Enterolactone & Enterodiols	Show weak estrogenic activity and help in hormone regulation
General Uses	Antioxidant, anti-inflammatory, anticancer, and antimicrobial

Commercial Applications

- Pharmaceutical Uses:
 - Podophyllotoxin is used as a starting material for anticancer drugs like *etoposide* and *teniposide*.
- Nutraceuticals:
 - Lignan-rich flaxseed and sesame are used in health supplements and functional foods.
- Cosmetic Applications:
 - Added to skincare products for antioxidant and anti-aging properties.

Tea (*Camellia sinensis*)

- Common Name: Tea
- Botanical Name: *Camellia sinensis* (L.) O. Kuntze
- Family: Theaceae
- Plant Type: Evergreen shrub or small tree.
- Origin: Native to China and Southeast Asia, now cultivated worldwide.
- Part Used: Young leaves and leaf buds.
- Significance: Tea is one of the most popular beverages in the world. It is known for its refreshing, stimulant, and antioxidant effects due to the presence of caffeine and polyphenols.



Composition

Tea leaves contain a variety of chemical constituents that determine its flavor, color, and health effects.

Constituent	Percentage/Function
Alkaloids (mainly Caffeine)	2–5%; acts as a stimulant
Polyphenols (Catechins, Tannins)	25–35%; antioxidant, gives astringent taste
Volatile Oils	0.005%; gives aroma and flavor
Amino Acids (Theanine)	1–2%; contributes to umami taste and relaxation
Pigments (Chlorophyll, Carotenoids)	Gives green color to fresh leaves
Minerals	Fluoride, potassium, manganese, etc.
Vitamins	Vitamin C, B ₂ , and folic acid

Chemistry & Chemical Classes

- Main Chemical Classes:
 1. Alkaloids: Caffeine, theobromine, theophylline (xanthine derivatives)
 2. Polyphenols: Catechins (epicatechin, epigallocatechin gallate - EGCG)
 3. Tannins: Theaflavins and thearubigins (formed during fermentation of black tea)
 4. Amino acids: Theanine – has calming effect

5. Volatile oils: Give pleasant aroma during brewing.
- Chemical Properties:
 - Caffeine: Mildly basic, soluble in hot water.
 - Polyphenols: Responsible for antioxidant and color properties.
 - Catechins easily oxidize to theaflavins (orange color) and thearubigins (brown color) during fermentation.

Biosources

- Botanical Source: Leaves of *Camellia sinensis*.
- Cultivation Areas: India (Assam, Darjeeling, Nilgiri), China, Sri Lanka, Japan, Kenya.
- Types of Tea Based on Processing:
 1. Green Tea: Unfermented leaves – rich in catechins.
 2. Black Tea: Fully fermented – contains theaflavins and thearubigins.
 3. Oolong Tea: Partially fermented – intermediate flavor and caffeine.

Therapeutic Uses

Constituent / Type	Therapeutic / Health Benefit
Caffeine	Central nervous system stimulant; reduces fatigue and increases alertness
Catechins (Green Tea Polyphenols)	Antioxidant, anti-inflammatory, anticancer activity
Theanine	Promotes relaxation, reduces stress
Fluorides	Prevent dental caries
Tannins	Astringent, helps in diarrhea
General Benefits	Improves digestion, boosts metabolism, protects heart and liver, may aid in weight management

Commercial Applications

- Pharmaceutical Uses:
 - Used in health supplements for antioxidant and weight-loss benefits.
- Cosmetic Uses:
 - Present in skin creams, anti-aging, and hair-care products for antioxidant effects.

Ruta (Ruta graveolens)



- Common Name: Rue, Garden Rue
- Botanical Name: *Ruta graveolens* L.
- Family: Rutaceae
- Plant Type: Small, aromatic, evergreen shrub.
- Origin: Native to Southern Europe; cultivated in India, Mediterranean regions, and North Africa.
- Part Used: Leaves and aerial parts.
- Description: The plant has bluish-green leaves, yellow flowers, and a strong aromatic odor.
- Significance: Used as a traditional medicinal herb for centuries — known for its antispasmodic, anti-inflammatory, and insect-repellent properties.

Composition

Ruta contains several active chemical constituents, mainly belonging to alkaloids, flavonoids, and essential oils.

Constituent	Type / Function
Alkaloids (e.g., Graveoline, Skimmianine)	Possess antispasmodic and antimicrobial activity
Flavonoids (Rutin, Quercetin)	Strengthen blood vessels, antioxidant
Coumarins (Rutamarin, Bergapten, Xanthotoxin)	Photosensitizing and vasodilator properties
Essential Oils (Methyl-nonyl ketone, Limonene)	Give characteristic odor; insect repellent
Tannins and Resins	Astringent and protective action

Chemistry and Chemical Classes

- Major Chemical Classes:
 1. Alkaloids: Quinoline and acridone type (e.g., graveoline, skimmianine)
 2. Flavonoids: Rutin, quercetin – known for antioxidant activity
 3. Coumarins: Rutamarin, bergapten – have phototoxic and vasodilator properties
- Chemical Nature:

- Most compounds are phenolic or aromatic in nature.
- Rutin (C₂₇H₃₀O₁₆) is a glycoside of quercetin and plays a major role in capillary strengthening.

Biosources

- Botanical Source: Leaves and aerial parts of *Ruta graveolens*.
- Geographical Source: Grown in India, Italy, Spain, France, and North Africa.
- Cultivation: Prefers warm, sunny climates and well-drained soil.

Therapeutic Uses

Ruta is widely used in traditional and modern medicine for various purposes.

Active Compound	Therapeutic Use
Rutin	Strengthens capillaries, reduces bleeding, and used in varicose veins
Graveoline and Skimmianine (Alkaloids)	Antispasmodic, anti-inflammatory, and analgesic
Coumarins (Rutamarin)	Used in vascular disorders, photosensitizing agent
Essential Oils	Used externally for insect repellent and muscle pain relief

General Pharmacological Actions

- Antispasmodic: Relieves muscle spasms.
- Antimicrobial: Effective against bacteria and fungi.
- Anti-inflammatory: Reduces swelling and pain.
- Antioxidant: Neutralizes harmful free radicals.
- Uterotonic: Stimulates uterine contractions (used traditionally, but not safe in pregnancy).
- Insect repellent: Due to strong volatile oil content.

Commercial Applications

- Pharmaceutical Uses:
 - Source of Rutin, used in preparations for capillary fragility, varicose veins, and hemorrhoids.
- Cosmetic Uses:

- Extracts used in skin and hair care for antioxidant and antimicrobial properties (in small amounts).

