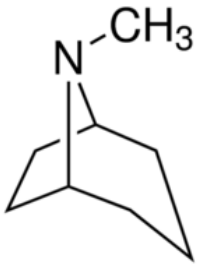
Chemotaxonomy

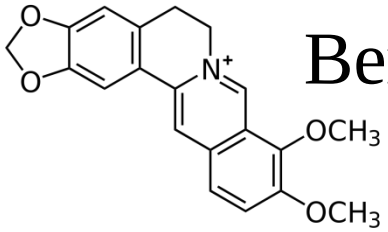
Chemotaxonomy :

This system relies on the **chemical similarity of taxon** (it is based on the existences of relationship betweens constituents in various plants). There are certain types of a **chemical constituent** that **characterize certain classes of plants**. This gives birth to entirely new concept of chemotaxonomy that **utilizes chemical facts** to understanding the taxonomical status, relationships, and evolution of plants.

For example :

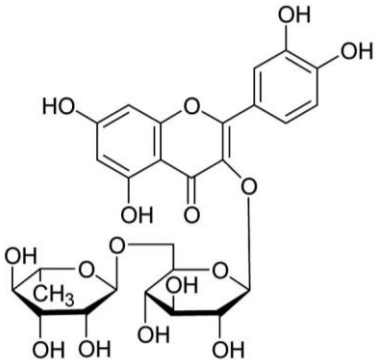


Tropane alkaloids: generally occur among the members of Solanaceae family.



Berberine alkaloids in Berberis and Argemon.

Rutin in Rutaceae



This system gives more scope for understanding the relationship between chemical constituents, their biosynthesis and their possible action

Chemistry of Natural Products

Natural drugs are divided into different groups according to the chemical nature of their most important constituent into the:

Primary metabolites

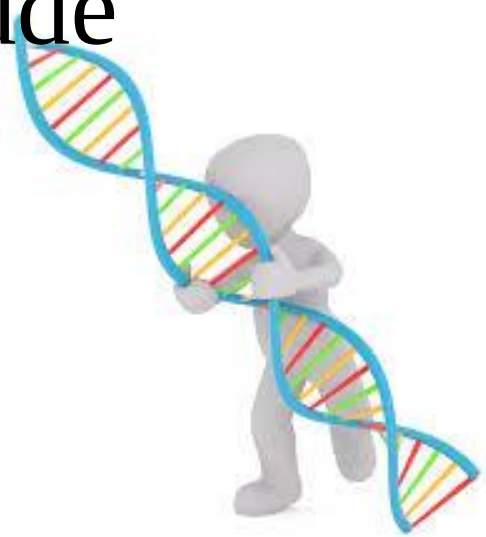
- Carbohydrates
- Protein

Secondary metabolites

- Glycosides
- Tannins
- Volatile oil
- Lipids
- Alkaloids
- Resins

Secondary metabolites are derived from primary metabolites

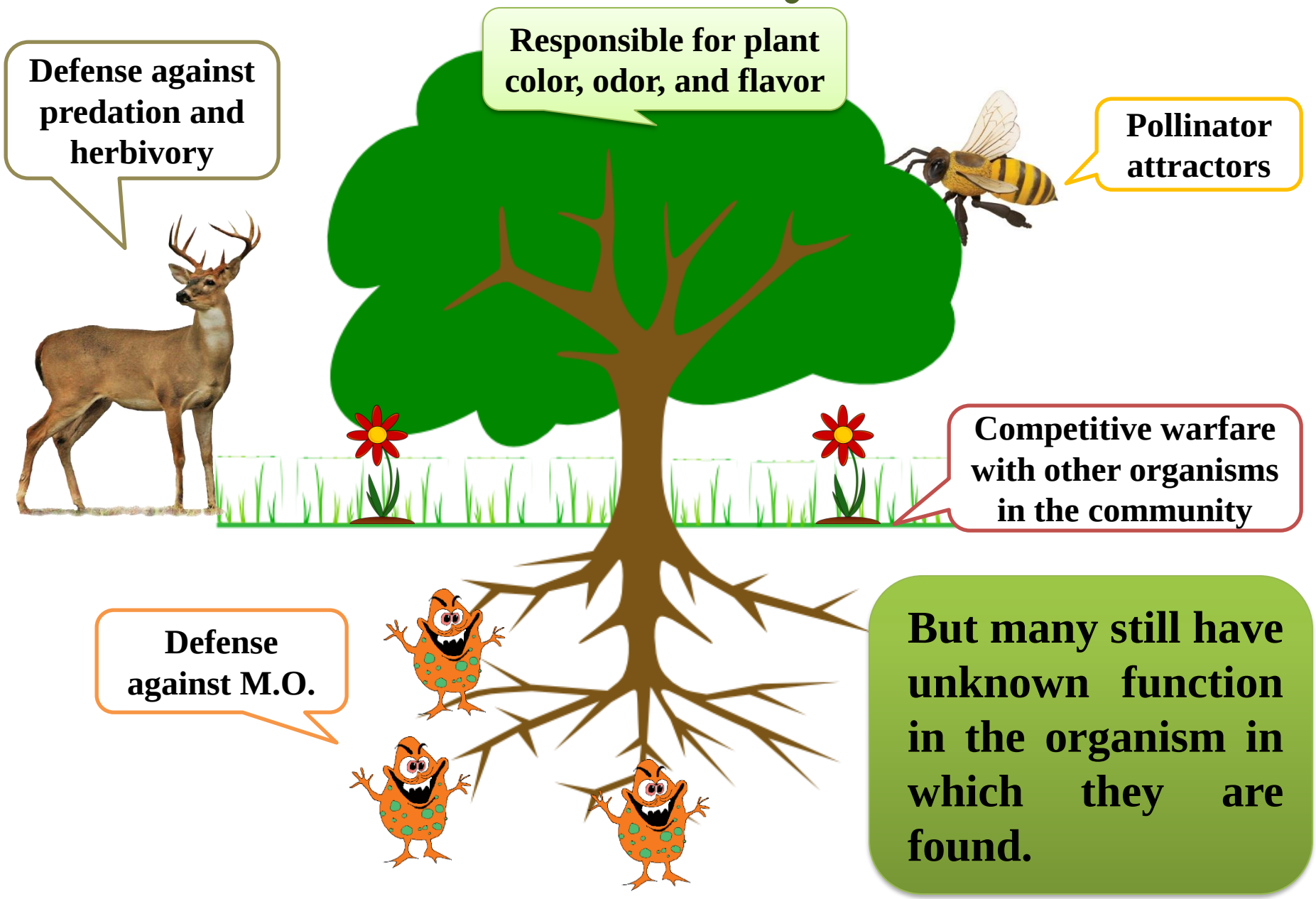
Primary metabolites: include the **nucleic acids** and the common **amino acids** and sugars. Secondly, there are the high-molecular-weight polymeric materials such as **cellulose**, the **lignins** and the **proteins** which form the cellular structures.



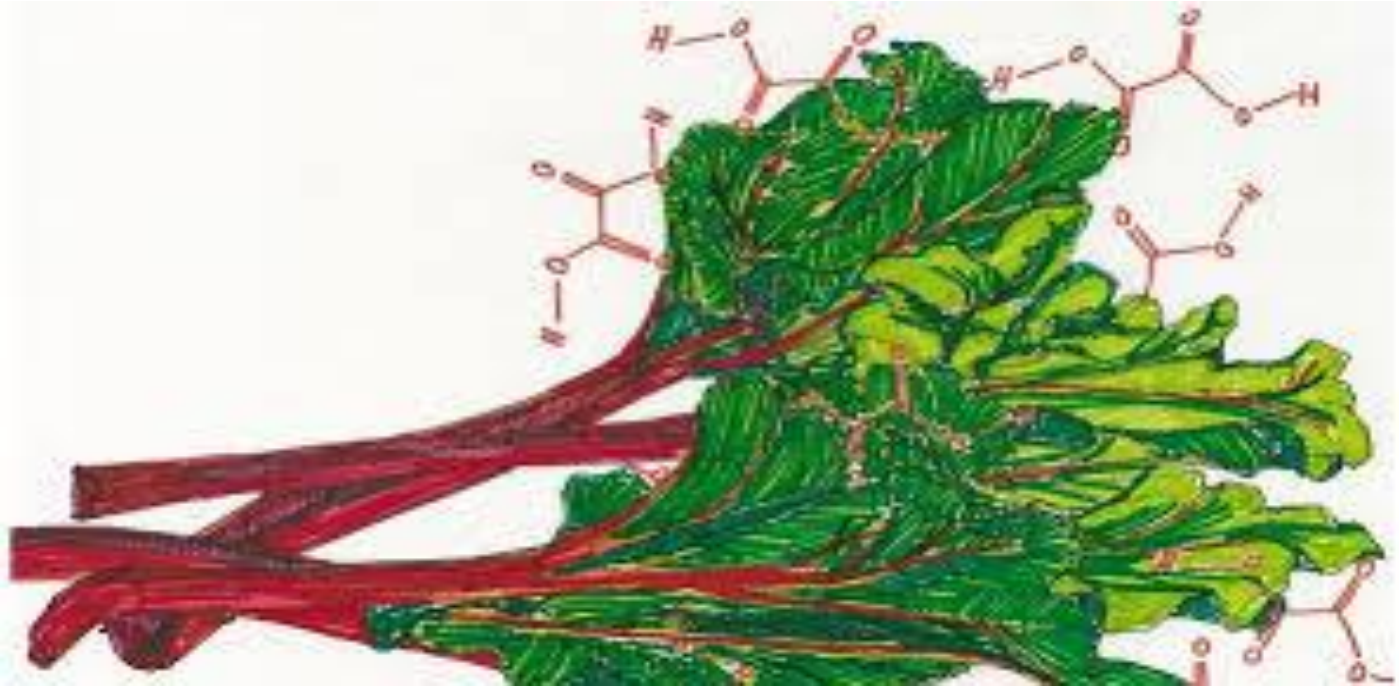
Secondary metabolites are those metabolites which are often produced in a **phase of subsequent to growth**, have **no function in growth** (although they may have survival function), are produced by certain **restricted taxonomic groups of organisms**, have unusual chemicals structures, and are often formed as mixtures of **closely related members** of a chemical family.

They have a wide range of chemical structures and biological activities. They are derived by **unique biosynthetic pathways** from primary metabolites and intermediates.

Function of Secondary Metabolites



Some families and its chemical characters



Solanaceae

comprised of some 2500 species, They have great value as food, like the well-known potato, tomato and eggplants, and medicines. The toxic species of this family are characterized by the occurrence of a variety of chemical compounds, for example:

- Tropane alkaloids (*Atropa* spp, *Datura* spp.)

- Glycoalkaloids, solanine (*Solanum* spp.)

- Nicotine (*Nicotiana* spp.)

Lamiaceae (Labiatae)

Sweet aromatic smell due to essential oils present in sessile glandular hairs. Terpene compounds were both qualitatively and quantitatively the major chemical group among the identified aroma compounds.

- *Mentha piperita*,

- *Lavandula angustifolia*

- *Salvia officinalis*.

Drug Deterioration

Several factors are to be considered for the detrimental effects on the natural drugs and this included:-

1)Primary factors

2) Secondary factors.

The factors which most to be considered in relation to drug deterioration are:

1) Moisture content

2) Temperature

3) light

4) The presence of oxygen.

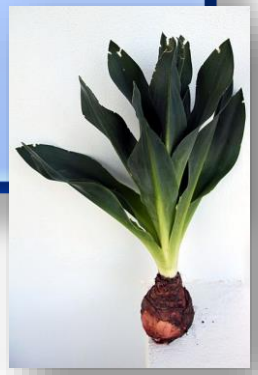
Primary factors

Primary factors:

1) Moisture content:

air-dried drugs contain about 10-12 % of moisture & in some cases (such as digitalis) this may be sufficient to activate the enzymes present in the leaves & this will lead to decomposition of the glycoside.

Other drugs such as powdered squill which contain mucilage quickly absorb moisture & become a sticky mass.



2) Temperature: An increase in temperature in combination with moisture may accelerate enzymes activity. e.g:

High temperature. Obviously those drugs containing volatile constituents in unprotected structures, e.g. plants belongs to Labiatae family and the petals of rose and chamomileall loose oil with an increase in temperature

3) Light: Direct sun light cause decomposition of certain constituents (e.g. vitamins in cod liver oil) as well as bleaching of leaves & flowers. In general, drugs should be protected by suitable light-proof wrapping or by the use of amber color containers. Powdered rhubarb stored in clear glass jars rapidly changes as the exposed surfaces turning from yellow to more reddish color.

4) Oxygen: presence of oxygen assists in the **resinification** of **volatile oils** & **rancidification** of **fixed oils.** Thus, these types of materials require storage in a well-filled, airtight container

Secondary factors

Living organisms usually develop in stored drugs where the conditions are satisfactory for them. From a hygienic point of view, such contaminated material should be destroyed irrespective of whether or not the active principles of drug have been affected. The more common of such organisms belongs to the groups of:

Moulds

Bacteria

Coleoptera or beetles

Arachnida

Secondary factors:

1) Moulds:

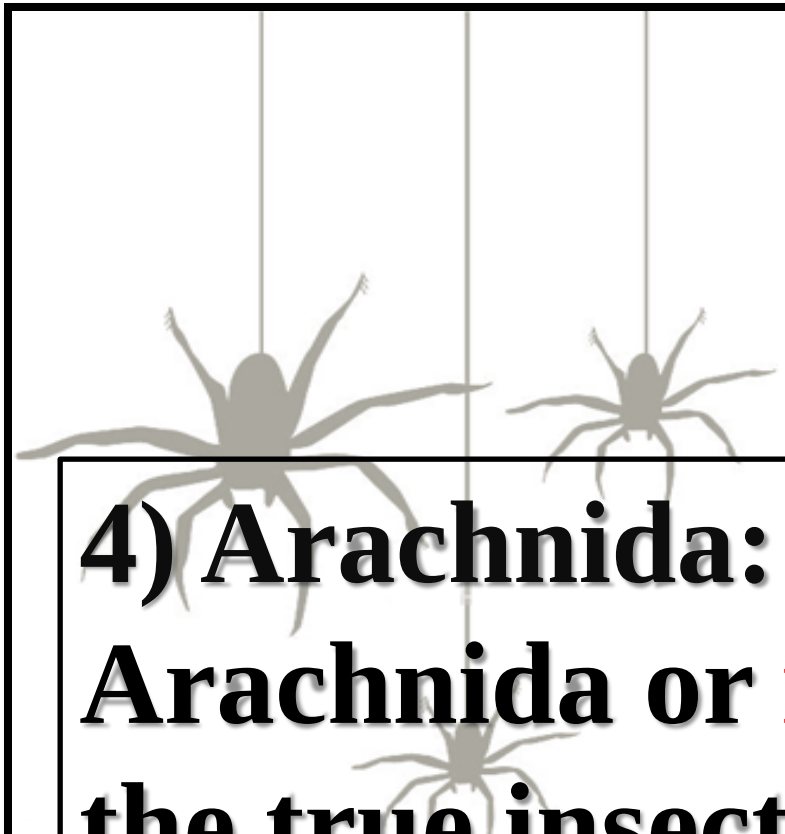
Moulds formed in the deteriorated drugs are usually the same as those associated with stored food products, the species of Rhizopus, Mucor, Penicillium & Eurotium are most common.

Their presence is indicated by a characteristic mass of hyphae & smell.

2) Bacteria: Bacterial attack of crude drug is less obvious but some pathogenic bacteria may be **tested** for **pathogenic** bacteria such as (Escherichia coli, Salmonellae) on some drugs taken internally as **digitalis**, **gelatin**, **tragacanth**.

3) Coleoptera or beetles:

Are insects which constitutes the largest order of animal kingdom & contains about 250,000 species of which 600 have been found associated with stored foods & drugs.



4) Arachnida:

Arachnida or mites differ from the true insects in that the mature forms have eight legs but possess no Antennae.


Drugs
Of
Evaluation

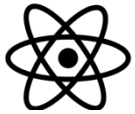
To evaluate a drug means to identify it &to determine its quality & purity, and this involves a number of methods:

Organoleptic

Microscopic

Biological

Chemical



Physical

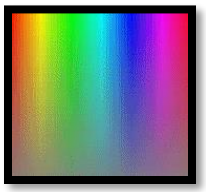
Spectral analysis

1) Organoleptic evaluation of a drug:

The majority of information on the identity, purity and quality of the material can be drawn from these observations, they are of primary importance before any further testing can be carried out, its refers to evaluation by means of organ of sense & include:

A) Shape & size

B) Color & external marking



C) Fracture & internal color

D) Odor & taste

2) Microscopic evaluation of a drug:

the microscope employed in the examination of drug. The microscope is not only used to study the

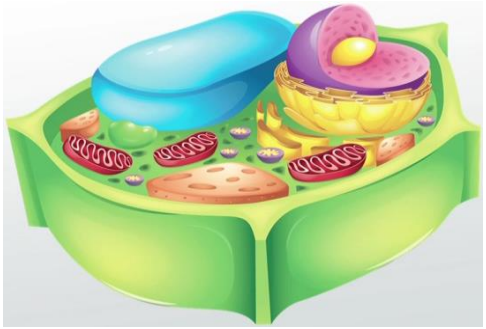
1) adulteration in the powdered plant or animal drugs.

but it is so important in the

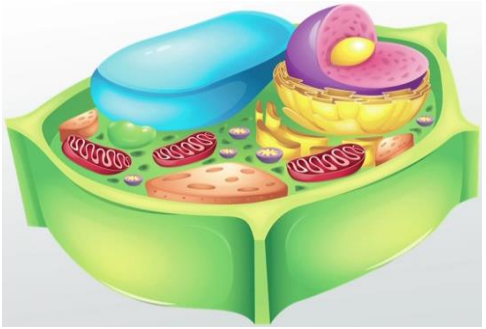
2) identification of pure powdered compounds.

Why we use Microscope??

- Powdered drugs possess very few macroscopic features with value in identification, so histological (microscopic) characteristic that are very important in the identification.
- The cells of powered drugs of being mostly broken that the content(like starch, lignin calcium oxalate crystals, fibers, .. ect) & scattered in the powder



Each cell has:



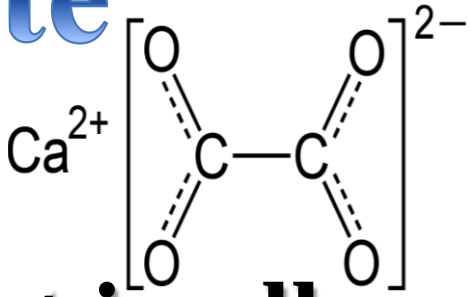
1) Fibers, vessels, stoma cells, trichomes, epidermal cells, stomata.

2) Cell contents & secondary metabolites.

1 & 2 called tissue elements

The presence or absence of these tissue elements which is seen under the microscope are used to determine the type of powdered drug.

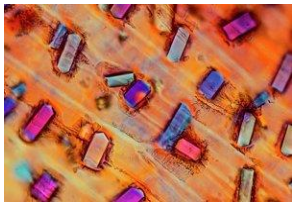
For e.g. calcium oxalate

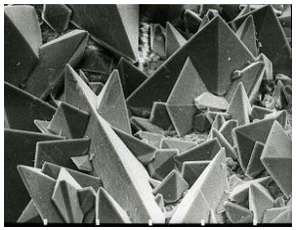


- **Ca is very important element in all cells rarely found in a free state but rather found as salts (like Ca oxalate, Ca carbonate)**
- **Ca salt (absorbed from the soil) + oxalic acid (produced as a result of metabolism).**

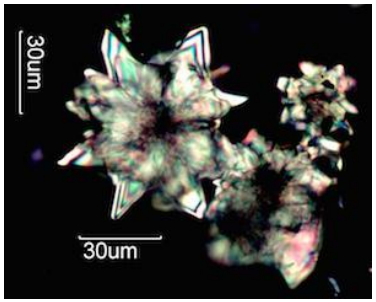
Calcium oxalate crystals appear as :

A) bundles of needles in onions.

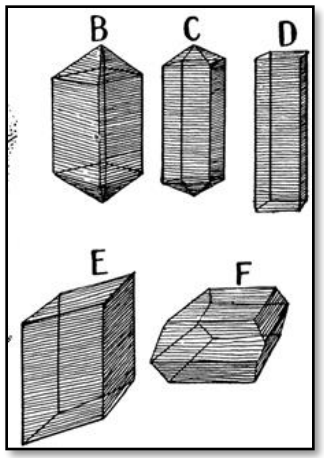




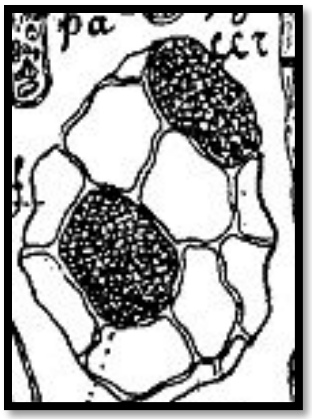
B) Star or flower shape (clusters) in Rhubarb



C) Crystal sheath (Prisms) in Liquorice & Senna.

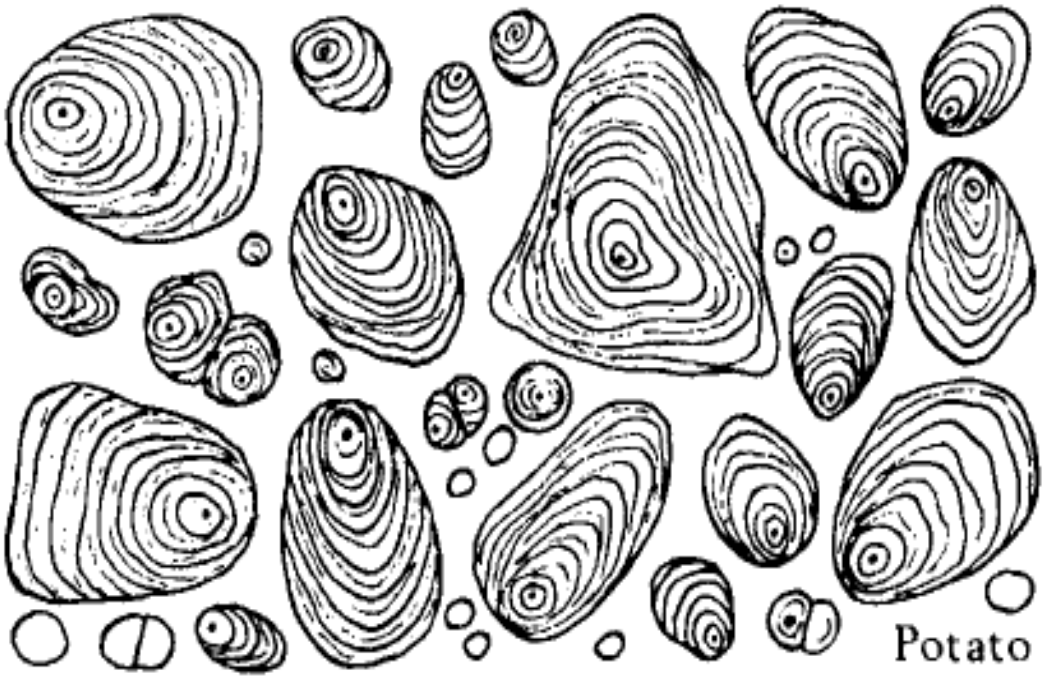


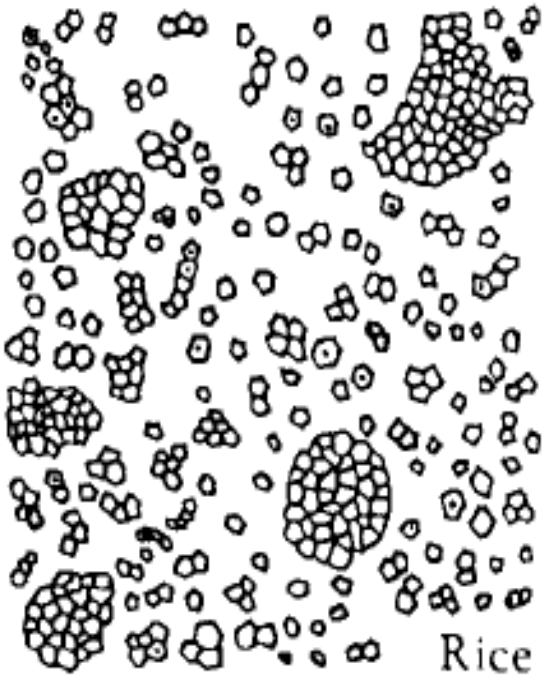
D) Microcrystals as in belladonna containing sandy crystals.

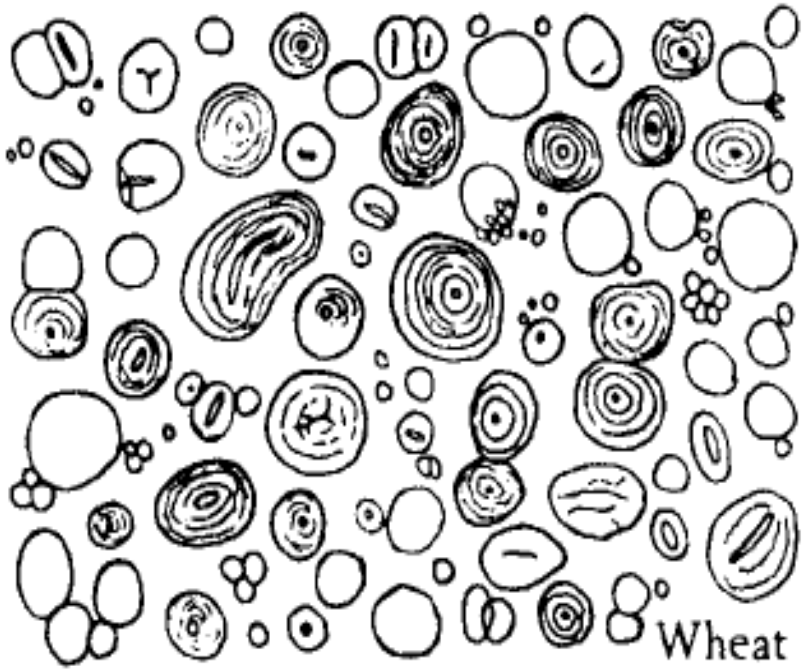


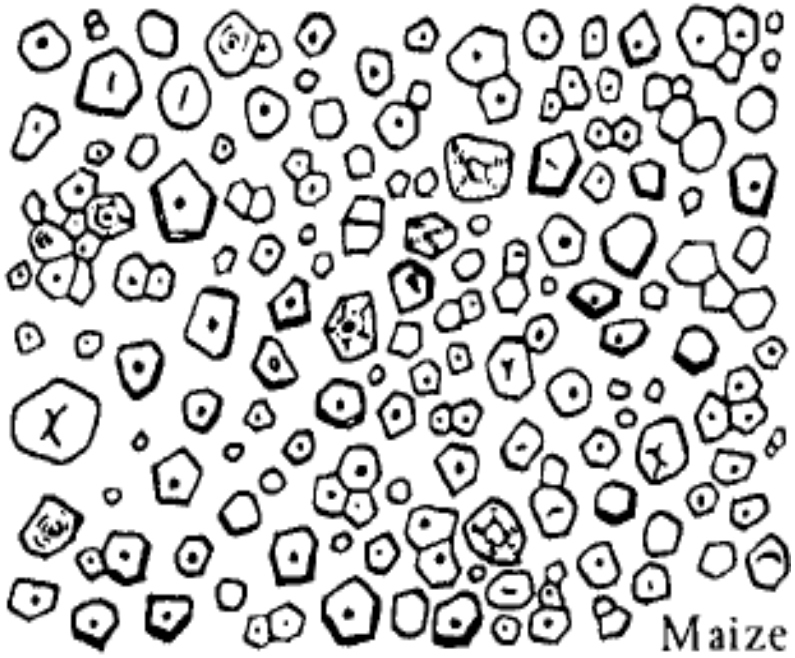
Other example is Starch

Starch have the same color & shape macroscopically but under the microscope we can differentiate between the different types of starch grains.


Potato


Rice

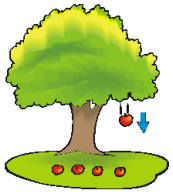

Wheat


Maize

3) Physical methods of evaluation

The physical properties that are employed for identification are:

Solubility



Specific gravity

Refractive index

Melting point

Water content

4) Chemical methods of evaluation of a drug:

By using chemical tests to evaluate crude drug (to determine the active constituents of the drug) by using chemical reagents in a colored reaction, such as:

1) Drug contain alkaloid → Dragendroff's → Orange to red color

2) Drug contain glycoside → KOH sol. 5% → Red color

3) Drug contain Tannins → $FeCl_3$ sol. → Green to brown color

These methods are used for Qualitative determination or Qualitative evaluation. While Quantitative determination using chemical methods involves the tests as in case of fixed oils

Acid value, iodine value..

5) Biological evaluation of a drug:

- **This evaluation include a range of pharmaceutical activity on living organisms, that is why it is called biological assay or bioassay.**
- **Other examples are: determination of antimicrobial activity of some drugs, antitumor activity, antioxidant activity, antifertility activity, hypoglycemic activity and neuro pharmacological activity .**

6) Spectroscopic or spectrometric method of evaluation:

This method can be used for evaluation of pure drugs or compounds from crude drugs.

spectrometric method

requires the isolation of the active constituent & then evaluate it by these methods (UV, IR, FT-IR, etc…..)

Example UV spectra for

Vincristine $\lambda_{max = 297\ nm}$

Vinblastin $\lambda_{max = 267\ nm}$


good luck on
midterms!