Summer Research Internship
Presentation On

# BIOLOGICAL TARGET MOLECULES AND LIGAND DATA SEARCH FOR MOLECULAR DOCKING EXPERIMENTS


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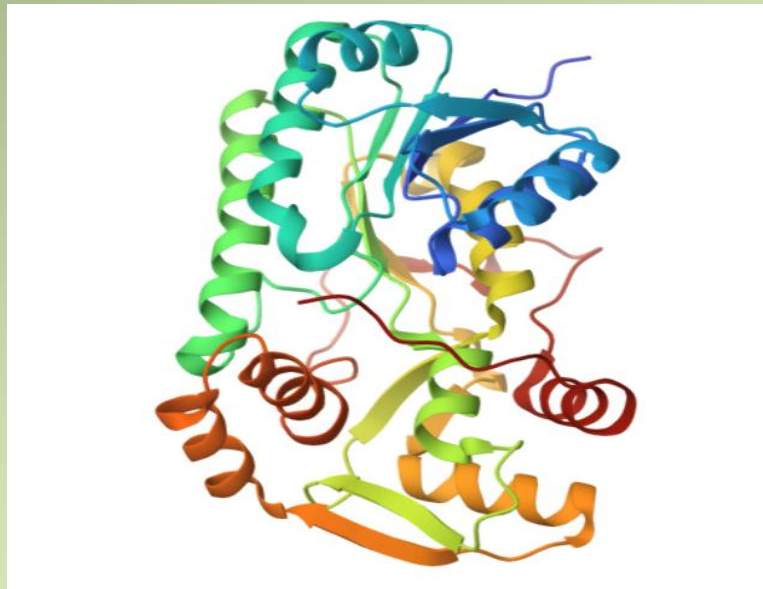
# ANTIBACTERIAL

# Introduction

- Phytochemicals, the bioactive compounds found in plants, play a vital role in combating bacterial infections.
- With increasing antibiotic resistance, exploring natural compounds as potential antibacterial agents has gained significant attention.
- This presentation highlights key research on antibacterial agents, including plant-derived constituents like those from Ocimum cufodontii and innovative materials such as Schiff bases and La-doped $CeO_2$ quantum dots.
- These studies emphasize molecular docking and spectroscopic techniques to uncover their mechanisms and potential applications in modern medicine

# Ocimum cufodontii



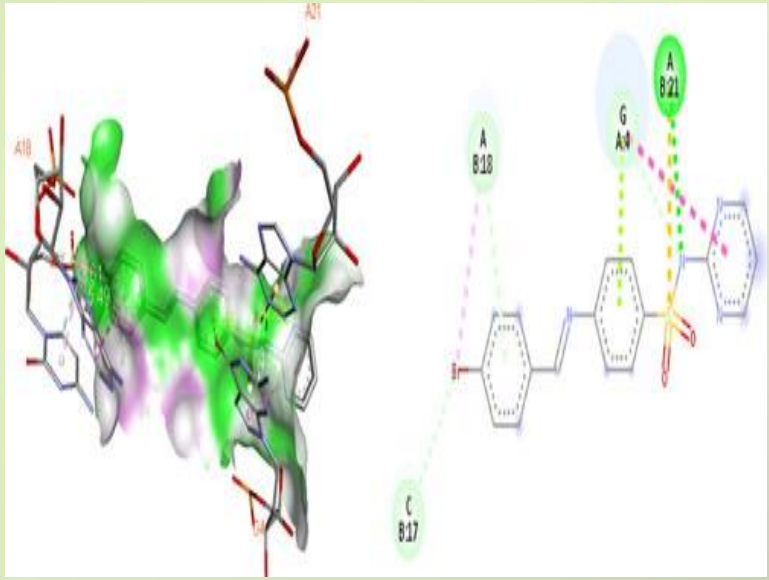
***Ocimum cufodontii***

- Tested antibacterial activity against *E. coli*, *K. pneumoniae*, and others.
- Molecular docking revealed interactions with DNA gyrase.
- Showed antioxidant activity (DPPH and FRAP assays.

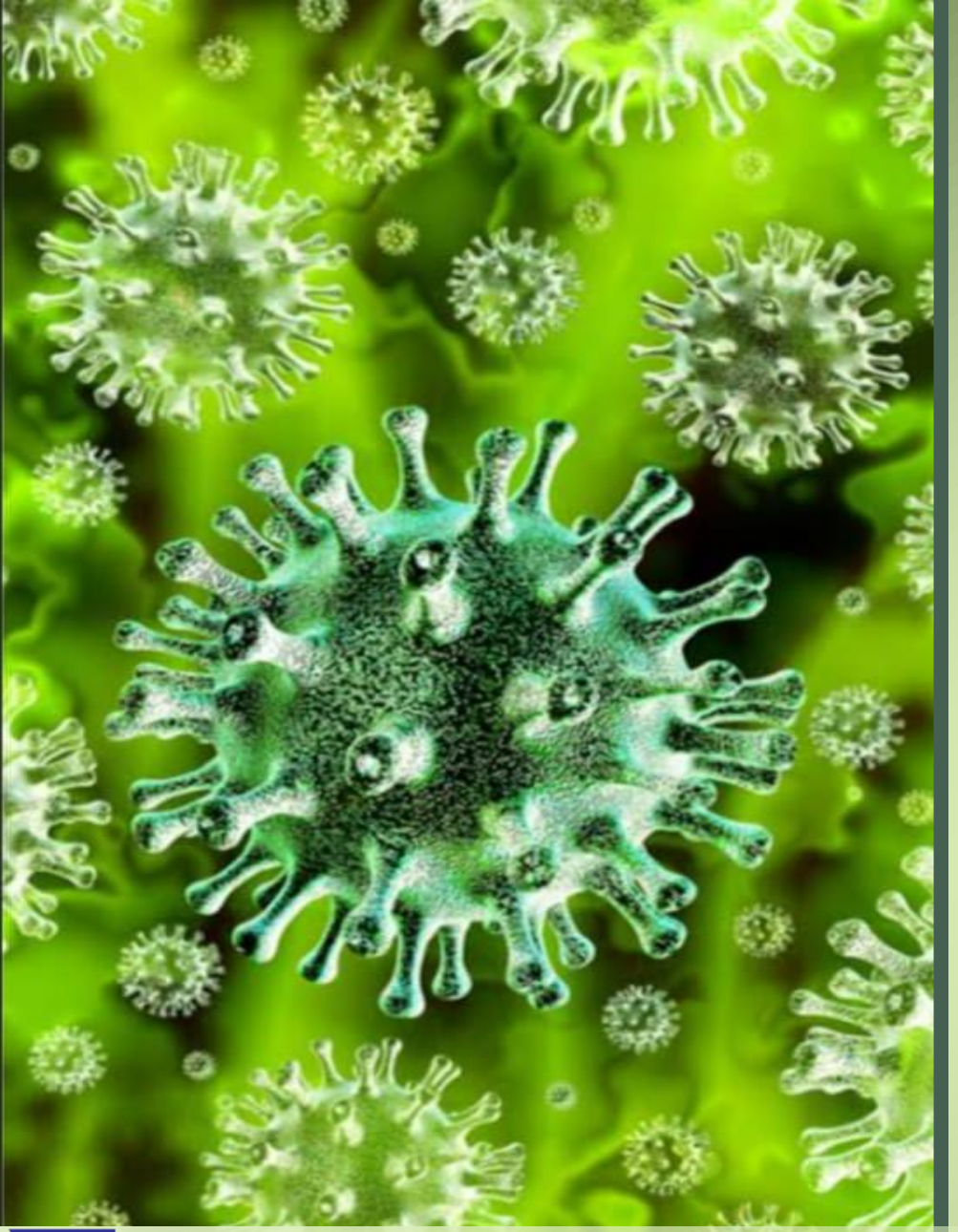
# Schiff Base Compounds

Synthesis and antibacterial potential of Schiff base (E)-4-((4bromobenzylidene)amino)benzenesulfonamide.

- Synthesized a novel Schiff base compound with characterization techniques (IR, NMR, UV-Vis spectroscopy).
- ADMET predictions and molecular docking validated its activity against *Staphylococcus aureus*.
- Strong antibacterial efficacy was confirmed.

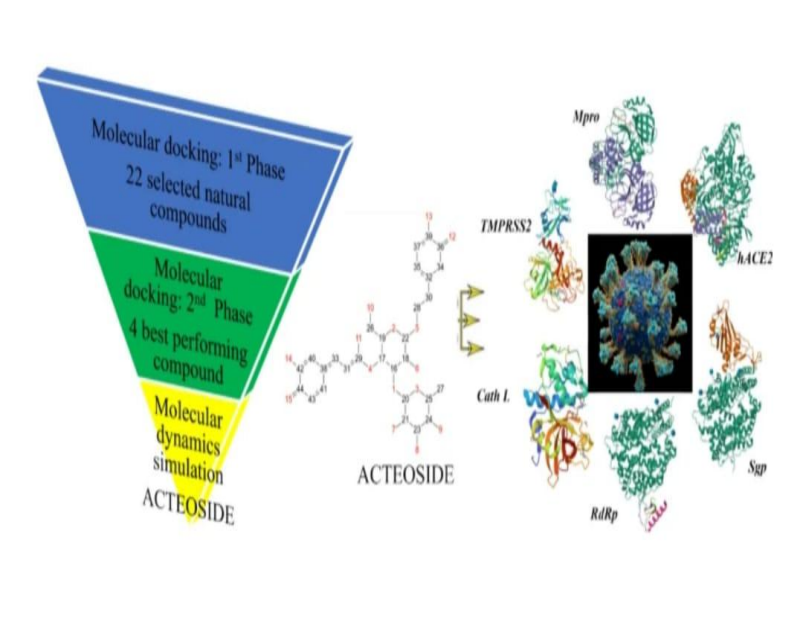


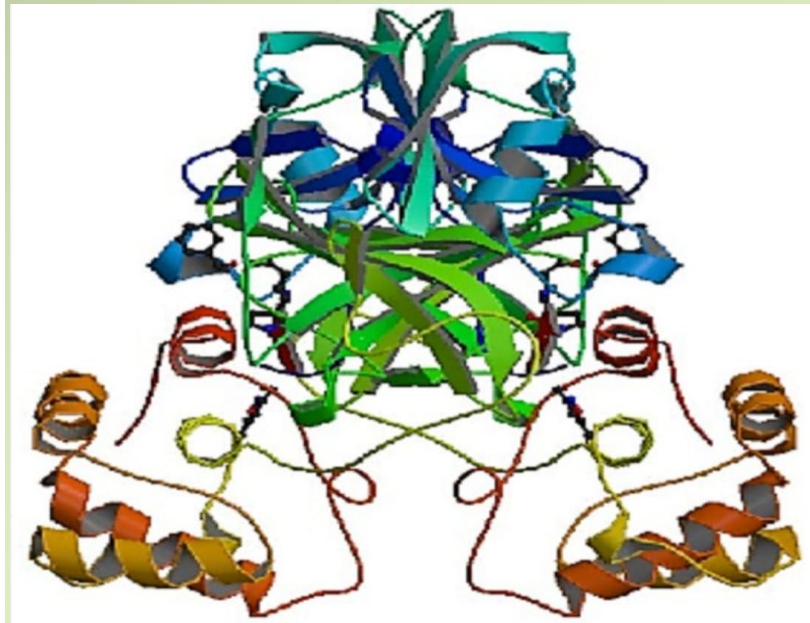

**(E)-4-((4-bromobenzylidene)amino) benzenesulfonamide**



# ANTIVIRAL

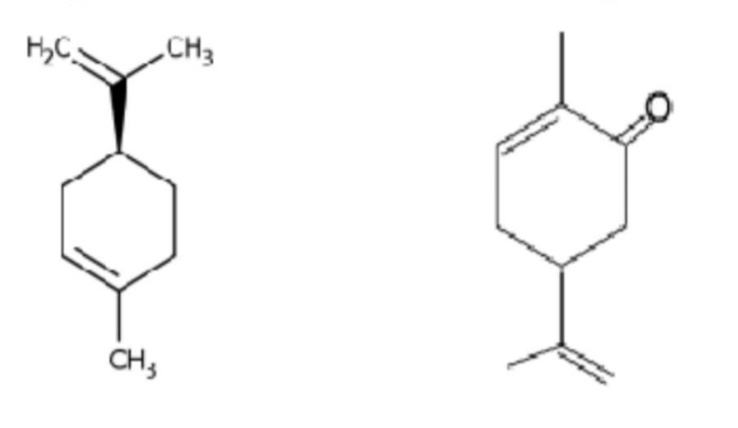
# 1. ACETOSIDE

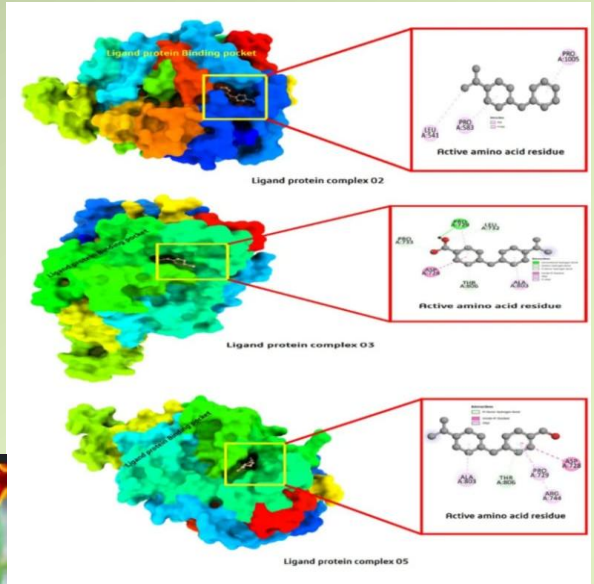


Acetoside, a natural compound found in various plants, has demonstrated potential antiviral activity against SARS-CoV-2. Molecular docking studies suggest that acetoside can bind to the main protease (3CL^pro) of the virus, inhibiting its replication.

# 2. LIMONENE DERIVATIVES




Protein–ligand interaction diagram and active site analysis. The Pink colour represent Pi-alkyl bonds, and the deep green colour hydrongen bonds.

Limonene derivatives have been studied computationally for their potential antiviral activity against the capsid protein of Herpes Simplex Virus-1 (HSV-1).

Docking studies indicate that these compounds may effectively bind to the viral protein, disrupting its function.

# 3. PEPTIDE BASED ANTIVIRAL AGENTS

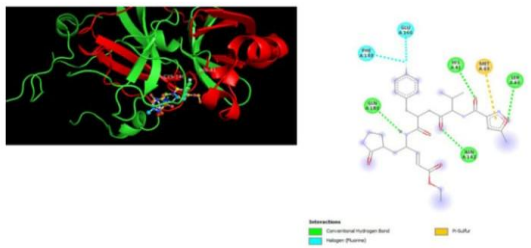


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*Figure 3.*
*The co-crystallized ligand rupintrivir with its 2D and 3D pose*

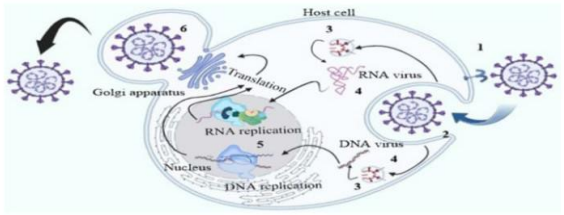


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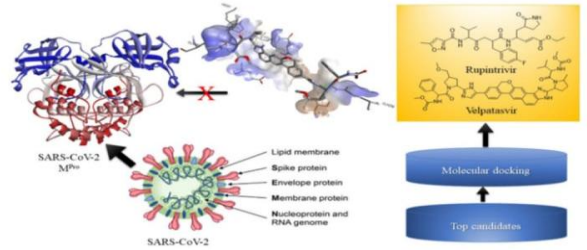
*Figure 1.*
*The antiviral peptides blocking sites of certain viral replication cycle. The inhibition sites are 1: viral association; 2: viral penetration; 3: endosomal escape; 4: viral uncoating; 5: viral genome replication; 6: release of mature virions*

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***Graphical abstract.***
*Affinity of viral protease inhibitors towards SARS-CoV-2 $M^{pro}$*

Peptide-based antiviral agents have been analyzed for their binding modes within the catalytic domain of the SARS-CoV-2 receptor. Molecular docking studies suggest that these peptides can effectively interact with viral proteins, potentially inhibiting viral entry into host cells.

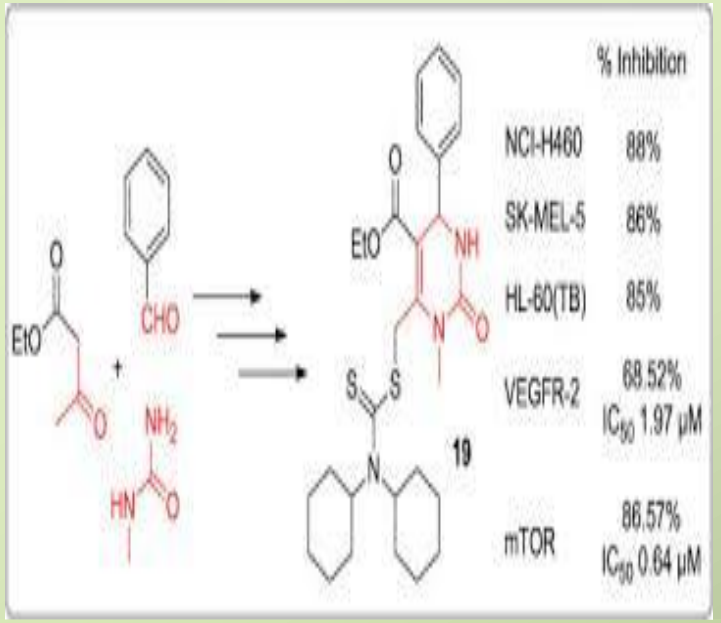

# ANTIDIABETIC

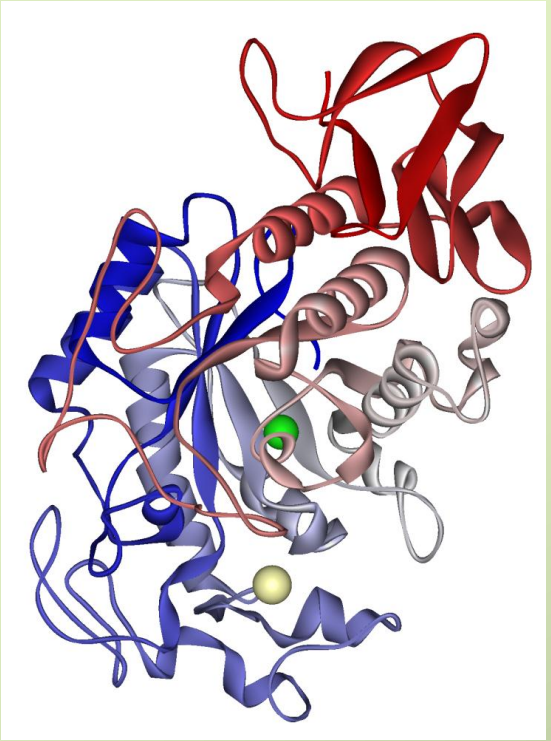
# *Dihydropyrimidinone Derivatives as α-Glucosidase and α-Amylase Inhibitors*

## Alpha-amylase

- An enzyme that breaks down starch and glycogen into smaller molecules like maltose and glucose.
- It's found in humans, animals, and plants.

Ligand: Dihydropyrimidinone



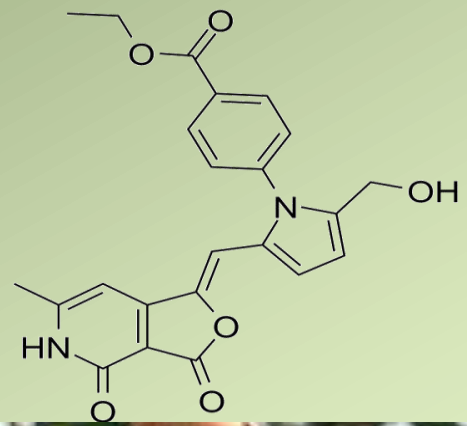



Protein target

*α-Amylase*

# *Bioactive Antidiabetic Flavonoids from Cordiadichotoma*

Protein target: α-Glucosidase,




Bioactive antidiabetic flavonoids from Cordia dichotoma exhibit significant potential in regulating blood glucose levels and improving insulin sensitivity. These flavonoids act by inhibiting key enzymes like a-amylase and a-glucosidase, reducing carbohydrate digestion and absorption. Their antioxidant properties further support the management of diabetes-related complications.

Ligands:Flavanoids from cordia dichotoma (Indian Cherry)

# ANTIFUNGAL

# Bioactive Compounds of *Acacia Concinna* against Fungal Protein

- **Bioactive Compounds**: Geranyl acetone, Trans-linalool oxide, Methyl salicylate, Cis-linalool oxide, 5-Methyl-2-furfural
- **Target Protein**: Candidapepsin-1
- **Ligand**: Geranyl acetone (highest binding energy)

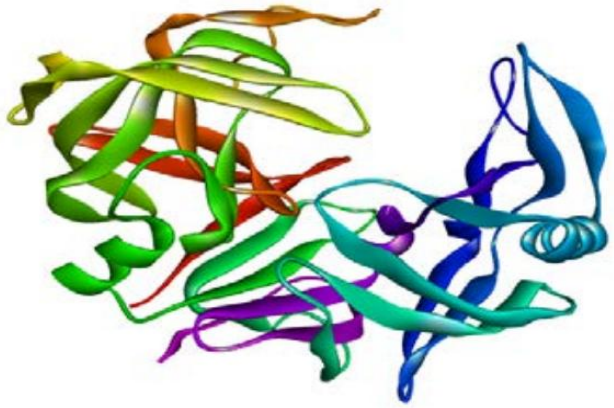
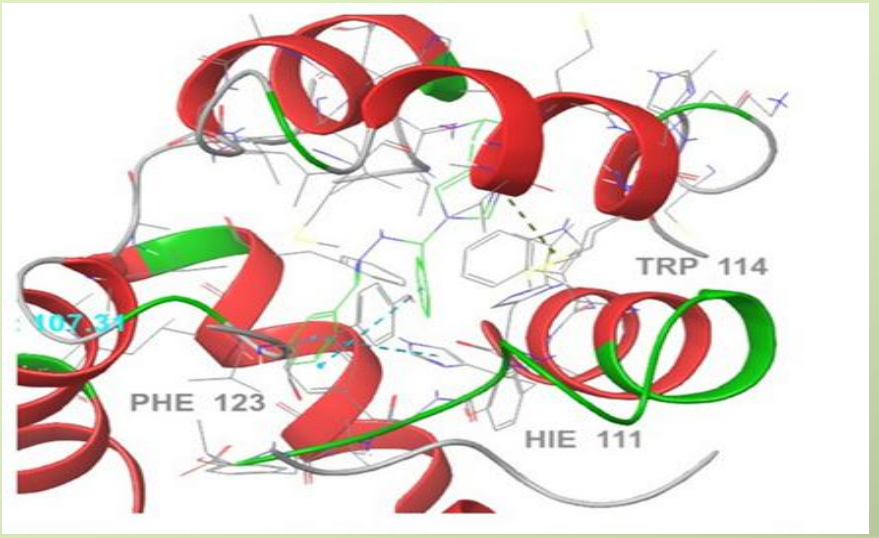


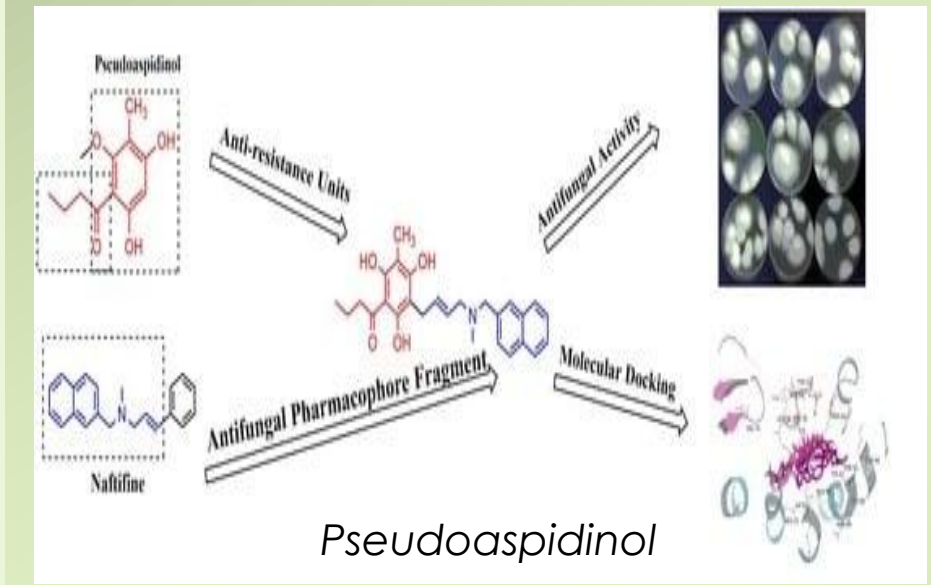
Figure 1: A chain amino acid of candidapepsin 1

***Shikakai***

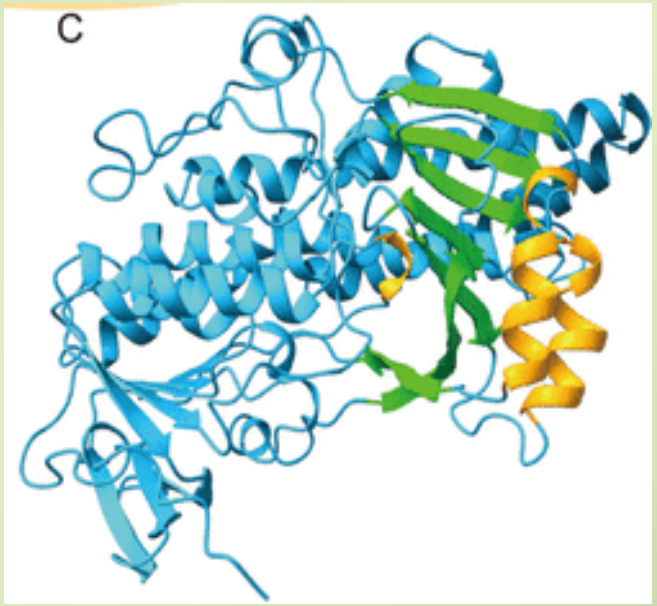


# Phluroglucinol derivatives

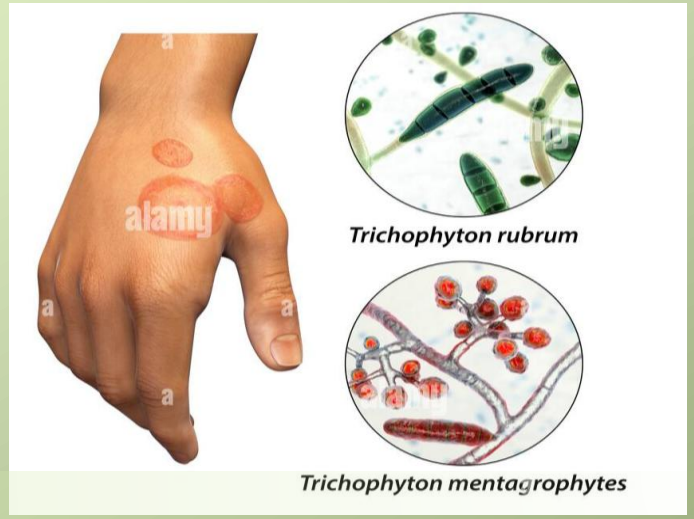
- ***Active Compound***: *Pseudoaspidinol (a phloroglucinol derivative).*
- ***Ligand***: *Phloroglucinol derivatives modified with allylamine and acyl groups.*
- ***Target Protein***: *Squalene epoxidase(involved in fungal cell membrane synthesis).*
- *Mainly targets* ***Trichophyton rubrum*** **and** ***Trichophyton mentagrophytes***




*Pseudoaspidinol*




***Target Protein***: *Squalene expoxidase*



# ANTICANCER

# Cancer: Target and Ligand Finding

**Cancer** is a group of diseases characterized by the uncontrolled growth and spread of abnormal cells.

Phytochemicals are natural compounds with therapeutic properties, including anticancer potential.

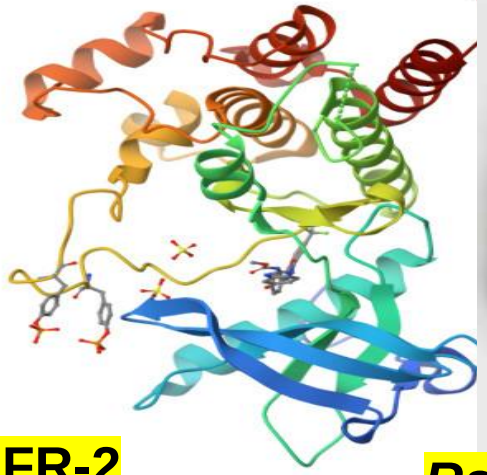
**Anticancer** refers to substances or treatments that can prevent, inhibit, or kill cancer cells.

Chemotherapy, Radiation therapy, Targeted therapy, Immunotherapy, Surgery etc…

Analysis of natural sources like plants and marine halophytes for anticancer compounds.

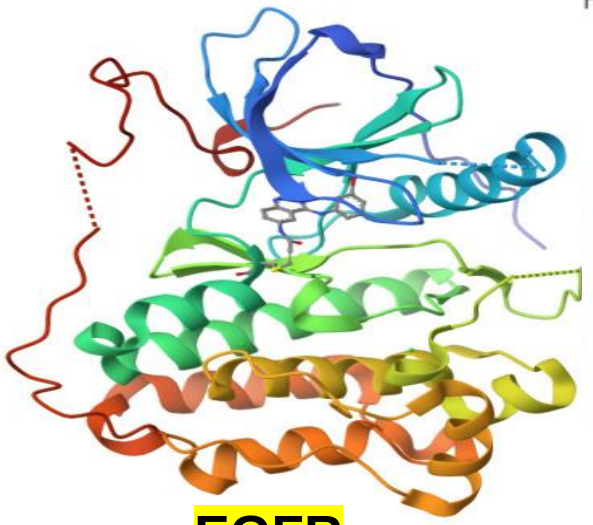
# Sources from Different Articles

- ***Raphia taedigera*** **Seed Oil (Ligands)**
  - **Targets Vascular Endothelial Growth Factor Receptor-2 (VEGFR 2)**
- ***Hepatocellular Carcinoma → 1000 Main (Liquoric Acid, Limonin etc)***
  - **Targets Epidermal Growth Factor Receptor and Caspase-9**
- **Marine Halophyte (*Suaeda maritima*)**
  - **CtBP1, SOX2**
- ***Parkia timoriana → 5 → Main (Oleic acid, +L Ascorbic Acid etc)***
  - **BCL-2, COX-2**

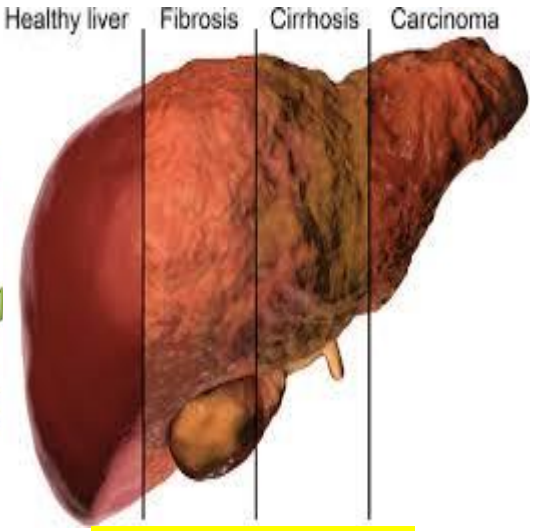


VEGFR-2

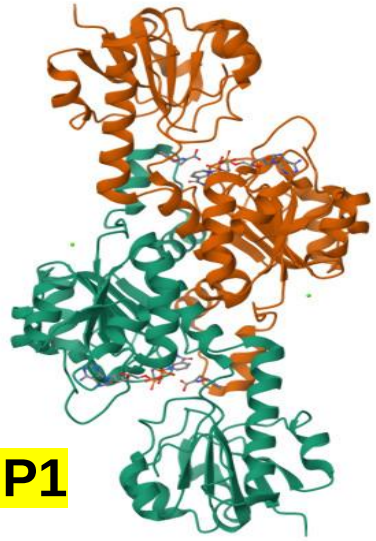
*Raphia taedigera* Seed Oil



EGFR

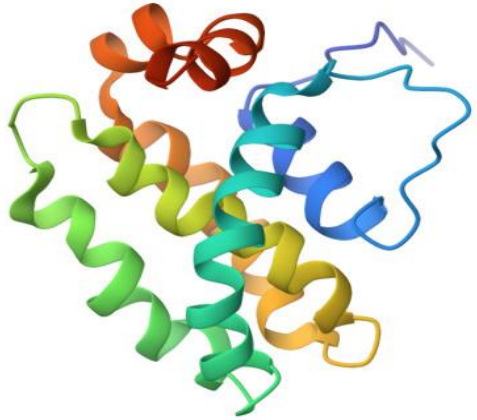



Liver Cancer



CtBP1

*Suaeda maritima*



Bcl-2

*Parkia timoriana*


ANTI-AGING

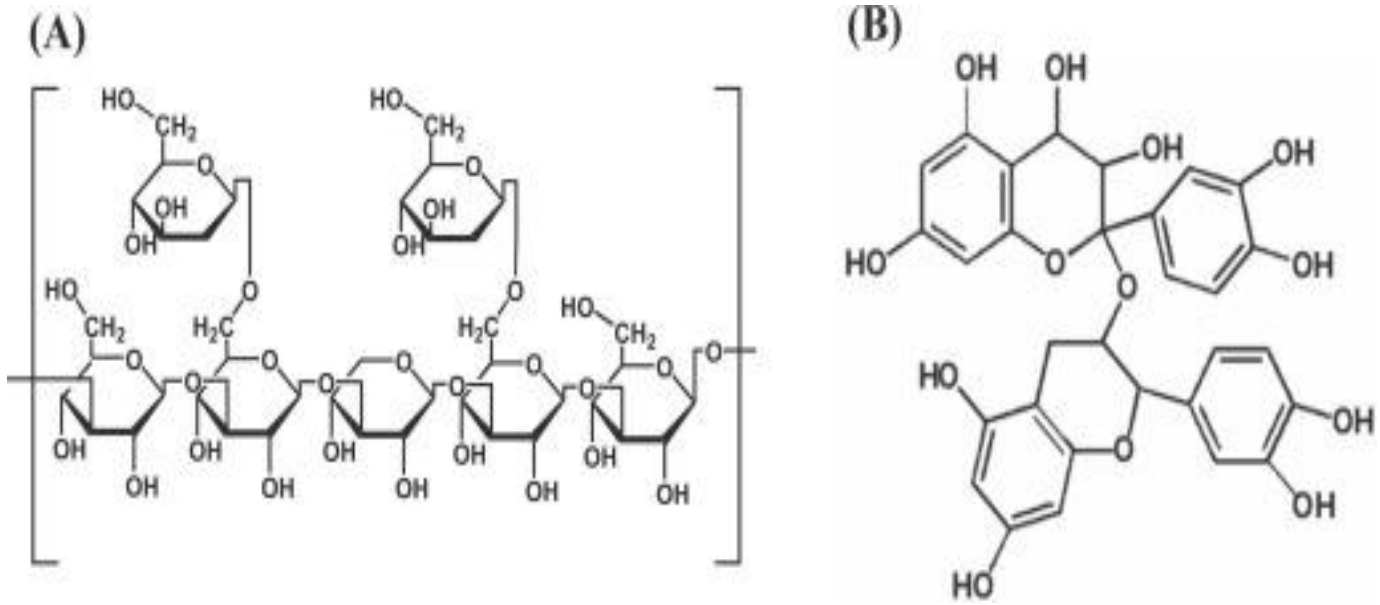
# RANBUTAN FRUIT EXTRACT IN AGING SKIN

- Anti-aging is the practice of using treatments or products to slow down the aging process.
- Rambutan fruits extract in aging skin
- Rambutan fruit peel extract has an anti-aging property due to presence of huge amount of polyphenolic compounds and is also proved that it can be used in the preparation of cosmetic cream.

# APPLICATION OF PLANT EXTRACTS COSMETICS IN THE FIELD OF ANTI-AGING

| | |
|---|---|
| **Moisturizing** | Aloe vera polysaccharide; Alginate; Tea polyphenols; Quercetin; Centella asiatica; Hyaluronic acid; Coconut oil; Jojoba oil |
| **Barrier repair** | Ceramide; Cholesterol; Sunflower seed oil; Walnut oil; Exotic oil; Grape seed oil; Safflower oil; Blackcurrant oil |
| **Anti-oxidation** | Proanthocyanidins; Resveratrol; Curcumin; Lactic acid; Salicylic acid; Catechins; Ginkgo flavonoid glycosides; Licorice flavonoids; Carotenoids; Astaxanthin; Vitamin C; Vitamin E; Coenzyme Q10 |
| **Sunscreen whitening** | Arbutin; Licorice; Glabridin; Anthocyanins; Lignin; Salidroside; Ascorbic acid |
| **Anti-inflammatory** | Curcumin; Nicotinamide; Lactobacillus fermentum; Grape seed oil; Proanthocyanidins; Squalene; Rose essential oil |

# STRUCTURES OF SOME COMPOUNDS




(A) Chemical Structure of Plant Polysaccharides;
(B) Chemical Structure of Proanthocyanidins.

Proanthocyanidins is a kind of polyphenol polymer, its phenolic hydroxyl group has strong hydrophilicity (as shown in (B), can maintain the water content of the stratum corneum, thus producing a moisturizing effect.

# References

***Research Articles:***


## *I. Anti-bacterial:*

1. *Synthesis, spectral analysis, antibacterial activity, quantum chemical studies and supporting molecular docking of Schiff base (E)-4-((4-bromobenzylidene) amino)benzenesulfonamide - ScienceDirect*

## *II. Anti-viral:*

1. *Molecular Docking Studies on the Anti-viral Effects of Compounds From Kabasura Kudineer on SARS-CoV-2 3CLpro – PMC*
2. *Ligand-based drug design against Herpes Simplex Virus-1 capsid protein by modification of limonene through in silico approaches | Scientific Reports*
3. *Molecular docking analysis of peptide-based antiviral agents against SARS-CoV-2 main protease: an approach towards drug repurposing*

## *III. Anti-diabetic:*

1. *Frontiers | Investigation of anti-diabetic potential and molecular simulation studies of dihydropyrimidinone derivatives*
2. *Bioactive Antidiabetic Flavonoids from the Stem Bark of Cordia dichotoma Forst.: Identification, Docking and ADMET Studies*

## *IV. Anti-fungal:*

1. *Molecular Docking Analysis of Bioactive Compounds of Acacia Concinna against Fungal Protein*
2. *Antifungal Agents: Design, Synthesis, Antifungal Activity and Molecular Docking of Phloroglucinol Derivatives*
3. *Dryopteris fragrans – Wikipedia*

## *V. Anti-cancer:*

1. *Phytochemical profiling, molecular docking, and ADMET evaluation of essential oils from Anaphalis busua and Anaphalis margaritacea in Uttarakhand's Himalayan Terrain – ScienceDirect*
2. *In Silico Molecular Docking of Bioactive Molecules Isolated from Raphia taedigera Seed Oil as Potential Anti-cancer Agents Targeting Vascular Endothelial Growth Factor Receptor-2 | Chemistry Africa*
3. *Molecular Docking and Simulation-Binding Analysis of Plant Phytochemicals with the Hepatocellular Carcinoma Targets Epidermal Growth Factor Receptor and Caspase-9*
4. *GC–MS and molecular docking analyses of phytochemicals from the underutilized plant, Parkia timoriana revealed candidate anti-cancerous and anti-inflammatory agents | Scientific Reports*

## *VI. Anti-ageing:*

1. *Application of plant extracts cosmetics in the field of anti-aging – ScienceDirect*
2. *Rambutan fruits extract in aging skin - ScienceDirect*


ANTI-BACTERIAL
ANTI-FUDTIC
ANTI-FUNGIC
ANTI-BACTERIAL
ANTI-BACTERIAL
ANTI-FUNGIC
ANTI-CANCER
ANTI-CANCER
ANTI-AGING
Thank You