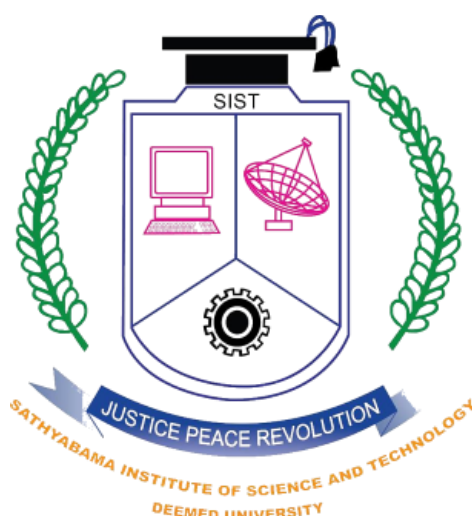


OPTIMIZING HYDROGEL FORMULATION FOR ENHANCED WOUND HEALING: INTEGRATING OF BIOACTIVE COMPOUND AND MECHANISTIC INSIGHTS

Submitted in partial fulfillment of the requirements for the award of
Bachelor of Technology degree in Biotechnology

By

SADHANA V (40230041)



**DEPARTMENT OF
BIOTECHNOLOGY**

**SCHOOL OF BIO AND CHEMICAL
ENGINEERING**

SATHYABAMA

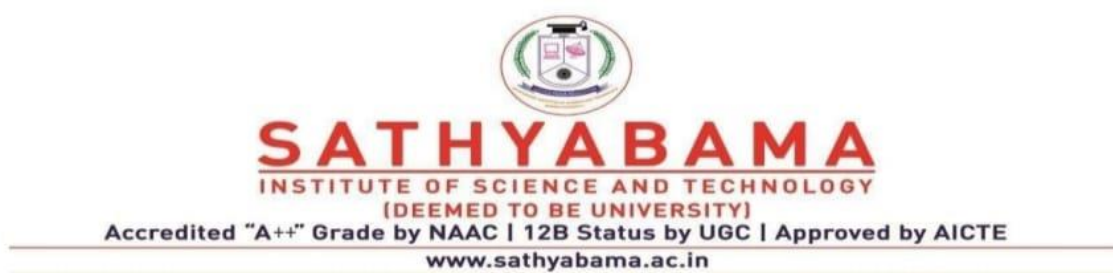
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BONAFIDE CERTIFICATE

This is to certify that this Review Report is the bonafide work of **SADHANA V (40230041)** who carried out Project Phase 1 entitled “**OPTIMIZING HYDROGEL FORMULATION FOR ENHANCED WOUND HEALING: INTERGRATING OF BIOACTIVE COMPOUND AND MECHANISTIC INSIGHTS**” under my supervision from June 2023 to April 2024.

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DECLARATION

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SADHANA V (40230041)

ABSTRACT

One of the major therapeutic and serious global health issue facing medicine today is wound healing. Lately, biocompatible and biodegradable materials have been combined to create wound dressings that enhance the healing process. Injecting hydrogels into the wound bed causes them to swiftly solidify into semisolid gels that cover the whole wound, shielding it from damage and absorbing secretions from the wound. Furthermore, hydrogels gradually introduce the medicine that has been encapsulated into the dermal wound because of their porous structure. One of the numerous benefits of using liposomes as a drug carrier for cutaneous wound healing is their capacity to carry both hydrophilic and hydrophobic medications. To improve drug-loaded liposome stability and lengthen the time the encapsulated medication is in contact with the skin, an matrix must be created because liposomes have a low viscosity and are consequently comparatively fragile. Dispersing the liposomes into a hydrogel, which may be employed as a platform for targeted distribution, is one method for getting around these problems. Therefore, the purpose of this work was to create encapsulated bioactive compounds in liposomes to optimize hydrogels formulation and examine how they may be used to treat dorsal full-thickness of excisional wounds.

Key words : Hydrogels, Wound healing, Bioactive compounds, Tissue regeneration, Scar minimization.

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LIST OF ABREVIATION

S.NO	ACRONYM	EXPANSION
1	SEM	Scanning Electron Microscopy
2	EPC	Phosphatidylcholine
3	OA	Oelic Acid
4	UV	Ultra violet visible spectroscopy
5	FTIR	Fourier Transform Infrared Spectroscopy
6	K _P	Kappaphycus
7	G _R	Gracilaria

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CHAPTER-1

INTRODUCTION

Wound healing is the process that involves the coordinated efforts of multiple cells, tissues, and biochemical pathways. In recent years hydrogel are promising features of wound healing because of unique features like gel structure , including their high water content, biocompatibility, and capacity to adapt to unusual wound geometries, have made them attractive materials for use in wound healing applications. However, hydrogel compositions must incorporate bioactive chemicals to maximize their therapeutic effectiveness. The integration has an opportunity to promote several facets of wound healing, including as tissue regeneration, antimicrobial activity, and anti-inflammatory actions. In addition, in order to optimize hydrogel-based dressing formulations and enhance therapeutic results, it is imperative to get mechanistic insights into the interactions between the dressing and the wound microenvironment. The initial step of improving hydrogel compositions for improved wound healing involves the meticulous selection and integration of bioactive substances capable of regulating crucial phases of the wound healing procedure. For example, it has been demonstrated that growth factors such as platelet-derived growth factor (PDGF) and epidermal growth factor (EGF) promote the migration and proliferation of different cells involved in wound repair, such fibroblasts and keratinocytes. Antimicrobial compounds, such as nanoparticles and antimicrobial peptides, have the ability to battle wound infections, which have been shown to obstruct the healing process. Through the incorporation of these bioactive substances into hydrogel matrices, scientists may fabricate multipurpose dressings for wounds that not only offer structural defense but also actively stimulate tissue regeneration and avert problems. Determining the right bioactive substances is just one thing to understand the mechanisms by which these substances interact with the wound microenvironment and to react. Examples of the results of research include the activation of downstream signaling pathways, such as the PI3K/Akt and MAPK pathways, by growth factors released from hydrogels. These pathways are essential for cell migration, survival, and proliferation.

Researcher concentrations and release kinetics of bioactive chemicals in hydrogels can be optimized to maximize therapeutic effectiveness by optimizing these mechanistic mechanisms. Moreover, mechanistic concepts may influence the creation of composite hydrogels that imitate the natural extracellular matrix and offer signals for tissue structure, cell adhesion, and differentiation all of which can eventually result in improved wound healing results

1.1 Phases of wound healing :

The human body has developed an incredibly complex mechanism to replace damaged tissue and return to normal operation. Wound healing may be broken down into several stages, each having unique traits and purposes of its own.

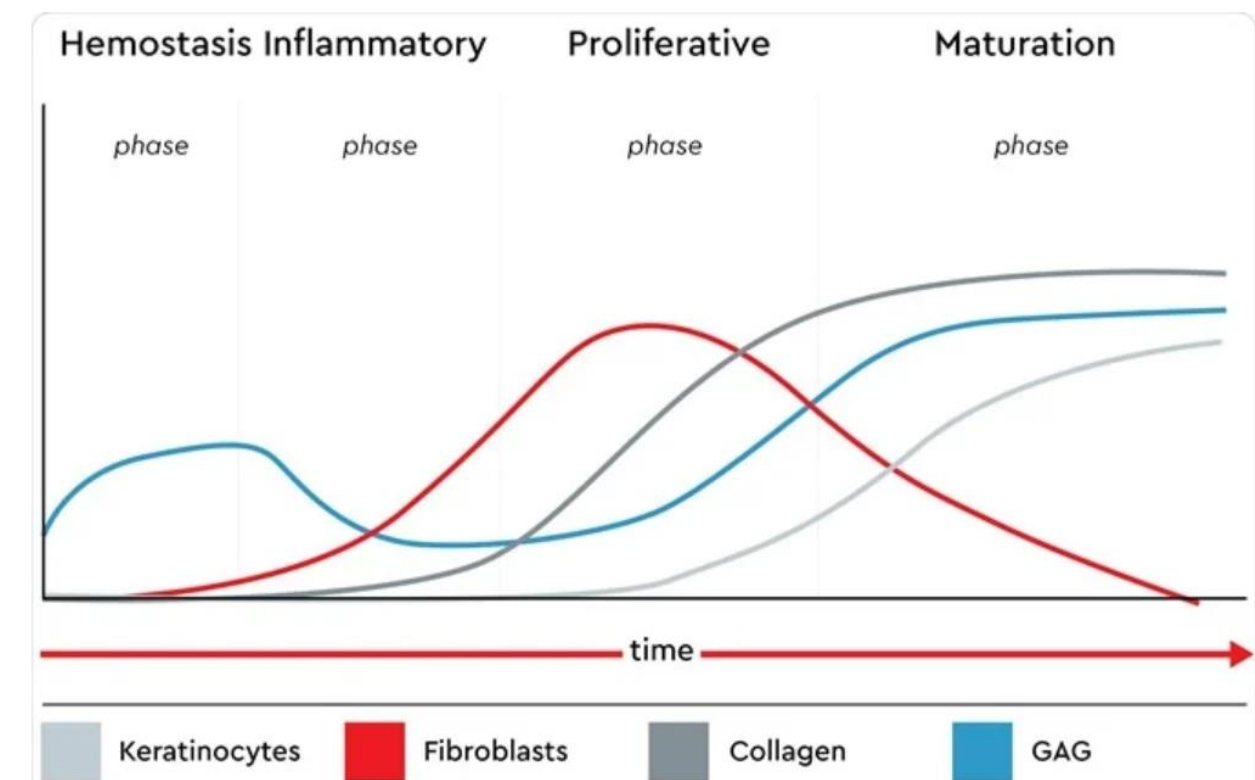


Fig 1.1 Four Phases of wound healing

Hemostasis, which includes the creation of new blood vessels to provide oxygen and vital nutrients to the wounded tissues, is an important step in the healing process of wounds. This complex system is essential to the body's ability to renew and mend damaged skin. Hemostasis facilitates the development of a network of blood vessels through a sequence of strictly controlled processes. This network is essential for the supply of growth factors, immune cells, and other elements required for appropriate wound healing. This procedure helps the healing process as a whole in addition to making tissue integrity repair easier. Hemostasis ultimately highlights the body's amazing capacity to organize a coordinated reaction to harm, resulting in the restoration of normal tissue function.

The inflammatory phase is the second stage of wound healing. This phase starts as soon as the damage occurs and is marked by the production of cytokines and histamine, which promote increased vascular permeability and local vasodilation. As a result, white blood cells—neutrophils in particular—flock to the injury site to remove debris and infections. In addition to preventing further tissue damage, the inflammatory phase also gets the wound ready for the next stages of healing.

The proliferative phase starts after the inflammatory phase. Numerous cell types, such as fibroblasts, endothelial cells, and epithelial cells, proliferate during this phase and cooperate to repair the injured tissue. Fibroblasts are essential for the production of new extracellular matrix, especially collagen, which gives the healing wound structural support. Angiogenesis, the process by which endothelial cells create new blood vessels, is crucial for supplying oxygen and nutrients to the healing tissue. Epithelialization is the process by which epithelial cells move from the borders of wounds to produce a new layer on the surface. All of these cellular processes work together to generate granulation tissue, which serves as the building block for the damaged tissue to begin to heal.

The remodeling phase is the last stage of wound healing. The newly produced tissue is remodeled during this phase to improve its strength and usefulness. To improve tissue strength, the original proliferative phase collagen fibers are rearranged and cross-linked. The scar tissue progressively grows and resembles the surrounding healthy tissue throughout this period, which can extend for months or even years. The remodeling phase tries to maximize the functional and cosmetic benefits of the healing process, even though scars may never be as strong or flexible as the original tissue.

1.2 LIPOSOMES :

Liposomes are spherical, tiny vesicles made of lipid bilayers that may encapsulate and transport many kinds of medicinal substances. Because these structures can protect and transport both hydrophobic and hydrophilic substances, they are used in the domains of medication delivery, cosmetics, and food technology. Liposomes are a desirable choice for targeted medication administration because they can be carefully manipulated to release their payload at particular places inside the body by careful adjustment of their composition and size. Their attractiveness in the pharmaceutical sector is further increased by their biocompatibility and capacity to imitate cell membranes. These lipid-based carriers continue to offer considerable promise for enhancing the safety and efficacy of a variety of drugs and therapies, thanks to continuous developments in liposome technology.

1.3 RED ALGAE STUDY :

Rhodophyta, another name for red algae, is a broad category of marine algae that is mostly found in tropical and subtropical areas' warmer coastal waters. They are an important part of marine ecosystems and are vital in giving different marine species a place to live and food. Red algae have also attracted interest due to its possible uses in a number of sectors, such as biotechnology, food, and medicine. Consequently, a great deal of research has been done to investigate the various facets of red algae, including their ecology, taxonomy, and possible industrial applications.

Red algae taxonomy and phylogeny are a pair of fields for research. Red algae represent a vast and varied phylum with more than 7,000 species now known to exist. Red algae are categorized by taxonomists into a number of orders, families, and genera according to their morphological, anatomical, and reproductive traits. Furthermore, new developments in molecular methods have shed light on the evolutionary connections between various red algae species. The previously mentioned studies have contributed to a better comprehension of the evolutionary trajectory and diversity of red algae, hence illuminating their ecological significance and capacity for environmental adaptability. From this red algae two types are algae used as therapeutic agent. One is Kappaphycus and another one is gracilaria.



Fig 1.3.1 Kappaphycus



Fig 1.3.2. Gracilaria

1.4 APPLICATION OF GELLAN GUM POWDER:

Gellan gum is a water-soluble anionic polysaccharide produced by the bacteria *Sphingomonas elodea*. It is commonly used in the food industry as a thickening, gelling, and stabilizing agent. Gellan gum has gained popularity as a vegan alternative to traditional gelling agents like gelatin and agar-agar. It is available in different forms such as gellan gum powder, gellan gum low acyl, and high acyl gellan gum. Each form has specific uses and applications in various industries.

Gellan gum powder finds application in the pharmaceutical sector as an emulsifying and suspending ingredient in topical gels, ointments, and oral drugs. It is the material of choice for pharmaceutical formulations because of its versatility and capacity to generate translucent gels. In addition to having a longer shelf life and greater stability than other gelling agents, gellan gum powder is a crucial component used in the manufacturing of pharmaceuticals.

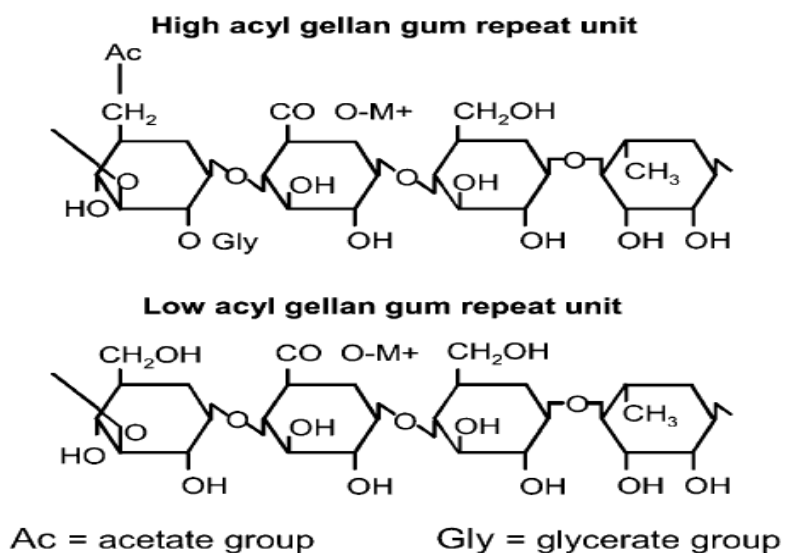


Fig 1.4 Structure of Gellan gum powder

CHAPTER-2

LITERATURE SURVEY

Wang et al. (2019) developed a bioactive self-healing antibacterial exosome hydrogel to aid in chronic diabetic wound healing and full skin regeneration. The study found that including bioactive molecules like exosomes into the hydrogel formulation greatly improved wound healing results, including increased antibacterial characteristics and full skin regeneration. This discovery stresses the need of including bioactive chemicals with wound healing properties into hydrogel formulations in order to maximize their therapeutic benefits.

In a similar vein, **Liang et al. (2022)** created pH/glucose dual-responsive metformin release hydrogel dressings that had adhesion and self-healing properties for sports diabetic foot wound healing. The study demonstrated the ability of dual-responsive hydrogel formulations to deliver bioactive substances such as metformin in a targeted and regulated way, promoting diabetic foot wound healing. This study's discovery emphasizes the relevance of mechanistic insights in the design of hydrogel formulations, particularly for bioactive chemical delivery in wound healing applications.

Moreover, **Huang et al. (2020)** announced the creation of a macroporous hydrogel dressing with improved antibacterial and anti-inflammatory properties to promote wound healing. The study highlighted the importance of integrating bioactive chemicals with antibacterial and anti-inflammatory characteristics into hydrogel formulations, which address essential elements of wound healing such as infection control and inflammation regulation. This research implies that combining bioactive chemicals with particular therapeutic processes might improve the design of hydrogel dressings for better wound healing results.

Gaspar-Pintiliecu et al. (2019) conducted a thorough evaluation of natural composite dressings based on collagen, gelatin, and plant bioactive substances for wound healing. The study emphasized the potential for natural bioactive chemicals, such as those derived from plants, to be included into hydrogel formulations to improve wound healing capabilities. This underlines the need for future study to investigate the various sources of bioactive chemicals and their mechanistic differences in order to better improve hydrogel formulations for wound healing purposes.

Melchels et al. (2014) investigated and characterized a novel bioink for additive tissue production. The researchers used gellan gum as the principal component of the bioink and proved its suitability for tissue engineering applications. Their findings emphasized the adaptability and tunability of gellan gum-based hydrogels, indicating that they are suitable for numerous tissue engineering applications.

Silva-Correia et al. (2013) investigated the biocompatibility of ionic- and photo-crosslinked methacrylated gellan gum hydrogels both in vitro and in vivo. The results showed that gellan gum-based hydrogels were highly biocompatible, making them interesting candidates for tissue engineering and regenerative medicine applications. The study's findings highlighted the promise of gellan gum hydrogels for in vivo applications, opening the door for future research into their long-term biocompatibility clinical translation.

Jaiswal et al. (2019) evaluated the potential of a carrageenan-based functional hydrogel film reinforced with grapefruit seed extract for wound healing applications. The study showed that carrageenan-based hydrogels had the capacity to cure wounds, showing that plant extracts can promote healing.

Li and Su (2018) explored smart hydrogels' multifunctional features, emphasizing its applications in tissue engineering and cancer treatment. While the study did not particularly focus on Kappaphycus extract, it did shed light on the broader applicability of hydrogels in wound healing and tissue regeneration, stressing the significance of natural plant-based materials in hydrogel production.

Sharaf and El-Naggar (2019) investigated the wound dressing capabilities of cationized cotton fabric treated with a carrageenan/cyclodextrin hydrogel infused with honey bee propolis extract. The findings showed that natural extracts have the ability to improve the qualities of hydrogel-based wound dressings, which supports the use of plant-derived materials in wound healing applications.

Yang et al. (2021) used photopolymerization to create a mussel-inspired adhesive, antioxidant, antibacterial, and hemostatic composite hydrogel wound dressing for infected skin healing. This work used bioinspired techniques to develop enhanced hydrogel wound dressings with adhesive, antioxidant, and antibacterial capabilities. The study's findings indicate that bioactive chemicals obtained from *Gracilaria* might be used into hydrogel dressings to improve their adhesion and therapeutic qualities for infected skin wound healing.

Li et al. (2020) developed a two-pronged technique for accelerating wound closure and healing using biomechanically active and biochemically multifunctional hydrogel wound dressings. This study concentrated on the multifunctionality of hydrogel wound dressings, highlighting the significance of biomechanical and biochemical aspects for improved wound healing. The findings highlight the potential of *Gracilaria* bioactive compounds to enhance the multifunctional properties of hydrogel wound dressings. Mussel-Inspired Adhesive Antioxidant Antibacterial Hemostatic Hydrogel.

Li et al. (2020) presented a two-pronged technique of biomechanically active and biochemically multifunctional hydrogel wound dressings to speed up wound closure and healing. This research demonstrates the possibility for combining mechanical and biochemical capabilities in liposomal hydrogel compositions to improve their efficacy in wound healing. The study emphasizes the need of using a diverse strategy when producing advanced wound dressings to improve clinical outcomes.

Albanna et al. (2019) used in situ bioprinting of autologous skin cells to expedite wound healing in large excisional full-thickness wounds. The study showed the promise of enhanced bioprinting techniques for wound healing. Future study might concentrate on improving the bioprinting method and better understanding the long-term consequences of in situ bioprinting on skin tissue regeneration.

Xu et al. (2020) reviewed the advancements and implications of antioxidant hydrogels for chronic wound healing. The study underscored the importance of hydrogels' antioxidant characteristics in facilitating wound healing in chronic situations. This discovery implies that the addition of Gracelaria bioactive compounds, which are renowned for their antioxidant characteristics, may improve the therapeutic potential of hydrogels for chronic wound treatment.

Liang et al. (2021) created dual-dynamic-bond cross-linked antibacterial adhesive hydrogel sealants for post-wound closure and infection healing. The study emphasized the importance of on-demand removability in wound care, which allows for sealant removal without injuring freshly produced tissue. This study found that liposomal hydrogel formulations have the potential to solve the issues associated with infected wound healing and post-wound closure.

Suarez-Arnedo et al. (2020) created an ImageJ plugin for high-throughput image analysis of in vitro scratch wound healing experiments. This application helps researchers quantitatively examine the impact of hydrogel treatments on cell migration and wound closure. However, further study is required to standardize the application of such image analysis methods across various experimental paradigms.

El-Kased et al. (2017) investigated the efficacy of a honey-based hydrogel for burn wound healing and found that it might promote tissue regeneration. This study focused on the therapeutic potential of natural hydrogel materials in wound healing applications. Future research might look at the underlying molecular and biochemical mechanisms of action for honey-based hydrogels in wound healing.

Fahimirad et al. (2021) found that liposomal curcumin released from 3D printed scaffolds had significant cytotoxicity against osteosarcoma cells while increasing osteoblast cell viability and proliferation, indicating the potential of liposomal formulations in wound healing and cancer therapy.

Briuglia et al. (2015) investigated the effect of cholesterol on liposome stability and in vitro drug release, which raises issues concerning the optimization of liposomal formulations to increase their stability and drug release kinetics for better wound healing results.

Furthermore, nanotechnology has been established as a viable technique for improving curcumin effectiveness and bioavailability in vivo (**Deshpande et al., 2016**). This study points to the potential of nanotechnology-based liposomal formulations to deliver curcumin and other medicinal compounds in wound healing applications.

Chen et al. (2019) studied the use of an injectable self-healing coordinative hydrogel to treat diabetic skin wounds. The results showed that the hydrogel has antibacterial and angiogenic characteristics, indicating that it might promote wound healing in diabetics. The study emphasizes the adaptability of hydrogel-based treatments and their capacity to address several elements of wound healing, such as infection control and angiogenesis.

Treesuppharat et al. (2017) created and studied a bacterial cellulose and gelatin-based hydrogel composite for drug delivery systems. The formulation had a lipid combination of DPPC, cholesterol, and DCP phospholipid in isopropanol. The study revealed the efficacy of this lipid combination in producing hydrogel composites with acceptable characteristics for drug delivery applications. The addition of lipid mixtures improved the mechanical strength and drug release characteristics of the hydrogel composite.

Sahraei and Ghaemy (2017) investigated the production of a modified gum tragacanth/graphene oxide composite hydrogel for heavy metal ion removal, as well as the development of a silver nanocomposite with antibacterial activity. The lipid combination used in this investigation consisted of N,N-methylene-bis-acrylamide and TiO₂ nanoparticles.

The researchers discovered that including this lipid combination resulted in the creation of a composite hydrogel with effective heavy metal ion elimination and antibacterial characteristics. The work demonstrated the use of lipid mixtures in customizing the functional properties of hydrogels for environmental and medicinal applications.

Aboelfetoh et al. (2017) showed the environmentally friendly production of silver nanoparticles using green algae, showing the possibility of combining algae-derived materials in hydrogel-based nanocomposites for a variety of catalytic and antibacterial applications. Furthermore, the use of hydrogels for protein detection has been investigated, demonstrating the flexibility of hydrogel-based systems in biological applications (Aboelfetoh et al., 2017). This highlights the potential for improving hydrogels made from red algae-derived materials for enhanced bioanalytical and diagnostic applications.

Chen et al. (2018) developed an ultratough, self-healing, tissue-adhesive hydrogel for wound dressings. This study's findings highlighted the importance of mechanical properties, self-healing ability, and tissue adhesiveness in designing hydrogels for wound healing applications, implying that these properties are critical for maintaining the integrity of the hydrogel dressing during the dynamic process of wound healing.

Larouche et al. (2018). Immune modulation of skin wound healing is an important element of the wound repair process, and recent research has shed light on the processes and new therapeutic targets involved. Understanding how immune cells interact with the wound microenvironment can help researchers create immunomodulatory techniques to improve wound healing results.

Sun et al. (2011) found that dextran hydrogel scaffolds increased angiogenic responses and facilitated full skin regeneration during burn wound healing. The work shed light on the potential of hydrogel-based scaffolds for wound healing and tissue regeneration. However, the particular processes governing angiogenic responses and molecular interactions between the hydrogel and host tissue are unknown, revealing a knowledge gap that requires additional exploration.

Fu et al. (2018). Fibroblasts are important participants in scar formation, and new research has found distinct fibroblast differentiated states that drive scar formation in the infarcted mouse heart. The 2,2-diphenyl-1-picrylhydrazyl (DPPH) test is commonly used to assess the antioxidant activity of different plant extracts. *Ageratum conyzoides* Linn., a plant species, exhibited high antioxidant DPPH radical scavenging activity, with an IC50 value of 24.8 µg/ml (semanticscholar.org).

Xing, Zheng, and Duan (2015) talked about two-photon polymerization microfabrication of hydrogels for tissue engineering and drug delivery. Gellan gum-based hydrogels might be investigated utilizing this cutting-edge 3D printing method. Future study might look at the usage of gellan gum in two-photon polymerization microfabrication to construct complex structures for tissue engineering and drug delivery.

Yegappan, Selvaprithiviraj, Amirthalingam, and Jayakumar (2018) investigated carrageenan-derived hydrogels for drug delivery, tissue engineering, and wound healing. Gellan gum-based hydrogels might be investigated for comparable purposes. Future study might compare the qualities and performance of gellan gum-based hydrogels to carrageenan-based hydrogels in order to determine gellan gum's distinct benefits.

Jiang, Chen, Deng, Suuronen, and Zhong (2014) addressed new platforms for drug delivery and tissue engineering, such as hydrogels. Gellan gum was not expressly stated, however it is known that it may be used to make hydrogels. Future study might focus on the development of gellan gum-based hydrogels for drug delivery and tissue engineering applications, as well as their potential benefits over other hydrogel forms.

Gupta et al. (2016) examined the creation, characteristics, and uses of nanoemulsions. However, gellan gum was not particularly highlighted in their research, indicating a possible knowledge gap in understanding its involvement in nanoemulsions. Future study might look at the possible usage of gellan gum in nanoemulsion formulations, as well as its effects on stability and drug delivery.

Shishir et al. (2018) reviewed current achievements in micro and nanoencapsulation of bioactive substances employing biopolymers and lipid-based transporters. The study stressed the potential of lipid-based transporters for encapsulating.

Zheng and Mcclements (2020) worked on developing more effective curcumin delivery devices utilizing colloid science. The study showed that lipid-based delivery systems can improve the solubility, stability, and bioavailability of curcumin, highlighting the adaptability of lipid mixture encapsulation for numerous bioactive chemicals.

Souza et al. (2011) studied the antioxidant capacity of two red seaweeds, *Gracilaria cornea* and *Gracilaria birdiae*, found on the Brazilian coast. Their analysis found IC(50) values of 0.86 and 0.76 mg mL⁻¹ for *G. cornea* and *G. birdiae* methanolic extracts, respectively. These findings indicate that red algal methanolic extracts have excellent antioxidant capabilities, making them promising candidates for the natural-antioxidant.

Marklein and Burdick (2010) described the production and characterisation of biocompatible PEGDA/Laponite nanocomposite hydrogels for 2D and 3D cell culturing.

Burdick and Prestwich (2011) examined the creation of hyaluronic acid (HA)-based hydrogels for biomedical applications, with an emphasis on the chemical crosslinking of pendant reactive groups. Burdick and Prestwich (2011) emphasized the utilization of addition/condensation chemistry or radical polymerization for crosslinking.

Tsuchiya, H. (2015) investigated phytochemical membrane contacts and molecular processes, but did not particularly address liposomal hydrogel formulations. This opens up the possibility of further study into the membrane interactions of bioactive substances inside liposomal hydrogel formulations, shedding light on their potential for targeted medication administration and controlled release.

Vos, W. D. de., Tilg, H., Hul, M. Van., and Cani, Patrice D. (2022) explored the gut microbiota and its relationship to health. However, the research made no mention of liposomal hydrogel formulations containing bioactive substances. This reveals a significant vacuum in the research about the possible influence of such formulation.

Ajeeshkumar, K. K., Aneesh, P., Raju, N., Suseela, M., Ravishankar, C. N., and Benjakul, S. (2021) discussed improvements in liposome technology and its applications in bioactive delivery. However, the precise use of liposomal hydrogel compositions including bioactive substances was not discussed. Future study might build on this analysis by investigating the efficacy of liposomal hydrogel formulations in delivering bioactive chemicals for better functioning and therapeutic results.

CHAPTER-3

AIM AND OBJECTIVE

3.1 AIM :

The aim of the research to develop and evaluate hydrogels for increased wound healing applications, with an emphasis on improving hydrogel formulations and integrating bioactive chemicals to promote efficient tissue regeneration and reduce scarring.

3.2 OBJECTIVE :

- Hydrogel formulation and optimization
- Incorporation of bioactive compound
- Characterization of hydrogel
- Mechanisms of action
- Document the experimental procedure, results, and analyses comprehensively.

CHAPTER-4

MATERIALS AND METHODS

4.1 MATERIALS:

4.1.1 COLLETION OF SEAWEED MATERIAL :

Red Seaweed are used in this study they are Kappaphycus and Gracilaria. These seaweed materials are produced from centre for ocean research, Sathyabama Reasearch park, Chennai.

4.1.2 CHEMICAL REQUIRED :

EPC, Oleic acid, Cholestrol, Chloroform, Phosphate buffer, Methanol, Gellan gum powder were purchased from Sigma Aldrich.

4.2 METHODOLOGY :

4.2.1. PREPARATION OF SEAWEED EXTRACT :

Extraction of each seaweed was prepared by pouring methanol into a bottle containing 50grams of seaweed powder at ratio of 10:1(v/w). After homogenisation; the mixture was kept under orbital shaking incubator at room temperature for 24 hours under dark conditions. Later, centrifuge 650g containing seaweed solution for 15 min to collect supernatant.

4.2.2 DPPH ASSAY RADICAL SCAVENGING ACTIVITY :

The Scavenging effect of crude methanol extract was determined by method of Yen and Chen (1995). The Scavenging activity of the seaweed extract Kappphycus and Gracilaria was determined by preparing a stock solution of 24 mg DPPH in 100ml of methanol and was filtered to obtain a unstable mixture with a absorbance at 517nm. The seaweed extract was measured by combining 3ml of the DPPH solution with 100µl of seaweed extract in a test tube. After incubation the tubes were kept in complete darkness for 30 minutes, the absorbance of the solution was measured at 517nm.

The Percentage of scavenging of DPPH radical was calculated by.

$$\text{DPPH scavenging effect (\%)} = [(Ac-As)/Ac]*100$$

Ac = Absorbance of control

As = Absorbance of sample

4.2.3. PREPARATION OF LIPOSOMES USING THIN FILM HYDRATION METHODS:

Preparation of liposomes was done by thin film hydration method. The mixture containing EPC: cholesterol: oleic acid was mixed at a ratio of 7.5: 1.5: 2.8 in 5ml of chloroform and was spread gently over the round bottom flask to obtain a thin film. Then the dried lipid mixture was rehydrated with 5ml of phosphate buffer saline and 1mg/ml of seaweed extract was added to lipid mixture. The resulting solution was vortexed for 1min and the multilamellar vesicles were obtained by sonication of lipid suspension for 3min. Ti probe sonicator was used to sonicate the multilamellar vesicles for 30s at 20w to produce unilamellar vesicles and filtered by polycarbonate membrane filter with 100nm pore size. (Fahimirad et al. (2021))

4.2.4 CHARACTERIZATION:

4.2.4.1 SCANNING ELECTRON MICROSCOPY:

Scanning electron microscopy (SEM) is a powerful imaging technique used to observe the surface topography and composition of a wide range of materials at a high resolution. This technique has revolutionized the field of microscopy by allowing for the visualization of micro and nanostructures in incredible detail. the fundamental principle of SEM lies in its use of a focused electron beam to interact with the specimen. When the electron beam is scanned across the sample's surface, various interactions occur, such as secondary electron emission, backscattered electron emission, and characteristic X-ray emission. These interactions are then detected and used to create an image of the specimen's surface, providing high-resolution, three-dimensional views of the sample. SEM can be used to analyze the chemical composition of a sample by employing energy-dispersive X-ray spectroscopy (EDS), which detects characteristic X-rays emitted from the sample and identifies the elements present.

SEM is also used to investigate the microstructure of materials, characterize nanostructured materials, analyze the quality of coatings and thin films, and study the morphology of nanoparticles

4.2.4.2 FTIR:

Fourier Transform Infrared (FTIR) spectroscopy is an effective analytical method that is used to determine and describe the chemical composition of a material. This technique is based on the principle that all molecules absorb infrared radiation at distinct frequencies, which can be used to identify functional groups present in the molecules. One of the key advantages of FTIR analysis is its ability to provide detailed information about the chemical structure of a sample. By measuring the absorption of infrared radiation at different wavelengths, FTIR spectroscopy can provide a fingerprint-like spectrum that can be used to identify the functional groups present in the sample. This information can be used to determine the molecular structure of the sample, identify unknown compounds, and monitor chemical reactions.

4.2.5 ENCAPSULATION EFFICIENCY :

The encapsulation efficiency (EE%) is defined as the ratio of the concentration of the integrated material (active substances, medicines, scents, proteins, insecticides, antimicrobial agents, and so on) identified in the formulation to the original concentration utilized to create the formulation.

The encapsulation efficiency (EE%) was determined using the formula below:

$$EE\% = (W_T / W_i) * 100\%$$

W_T = Total amount of integrated material

W_i = Total amount of incorporated material added at the start of the preparation.

4.2.6.LIPOSOMAL HYDROGEL FORMULATION USING GELLAN GUM POWDER

Gellan gum is a natural polysaccharide extracted from a specific type of bacteria *Sphingomonas elodea*. The gellan gum powder (0.2% w/v) was added in 100ml of double distilled water at 30mins by continuous stirring, cooled at 50°C and add the seaweed extract powder (1mg/g) was added and kept for 20min. The lipid suspension was gently mixed with gellan gum solution. (Melchels et al. (2014))

4.2.7.VISCOSITY OF HYDROGEL :

The high acyl gellan gum powder is used to make gel. For this viscosity test sodium chloride, potassium chloride, and calcium chloride is used for testing viscosity of gellan gum gel. The first step was to prepare gellan gum gel by magnetic stirring in 85°C for 30mins. After stirring, gellan gum powder dissolved in distilled water and form thick and milky fluid.

When the solution cools, it thickens and forms a soft gel that breaks down with agitation and mixing. Secondly, the effect of GLG concentration on viscosity was examined by adding GLG to distilled water at different doses. Thirdly, high temperatures were applied to GLG solutions in order to evaluate the impact of temperature on viscosity. Fourthly, the effects of monovalent and divalent ions on viscosity were measured by adding NaCl, KCl, and CaCl₂ to GLG solutions. Thus the viscosity GLG is measured by this method.

4.2.8 GELATION TEMPERATURE AND TIME :

Gellan gum hydrogels still face a significant challenge when it comes to encapsulating live cells in a tissue engineering setting while preserving their injectability. (Melchels et al. (2014)) for injectable encapsulation, the T_{gelation} is commercially available, that intact gellan gum is too high (> 42 °C) under physiological cationic circumstances to suspend cells. There are just a few appropriate chemistries and formulations since cells are present during the gelation process. Several studies on gellan gum hydrogels show that the gelation temperature may be adjusted to be medically appropriate by: (i) Adjusting gellan's molecular weight and (ii) functionalization of gellan with carboxymethyl and thiol groups.

CHAPTER-5

RESULTS AND DISCUSSION

5.1 EXTRACTED SEAWEED SAMPLE :

Plant extracts after centrifugation for 15mins.



Fig 5.1.1 plant extracts

In this fig 5.1.1 show the two type of methonolic extract shown one is kappaphycus and another one is gracilaria red seaweed which play important role in synthesis of liposome by enacapsulation method. This two type red algae has rich nutrient content which make base for hydrogel formulation with gellan gum powder. After extraction of this two extract lyophilisation is done which convert liquid solution into powder form which very useful to synthesis of liposomes by encapsulation method. Previously Jaiswal et al.2019; reported where the extraction of carrageenan which useful for hydrogel formulation.

5.2 DPPH ASSAY :

Table 5.2 Standard value of ascorbic acid and scavenging activity

S.no	Concentration (µg/ml)	Absorbance	Blank	%RSA
(1)	25	0.096	0.52	33.53
(2)	300	0.072	0.52	38.15
(3)	350	0.049	0.52	42.19
(4)	400	0.035	0.52	45.26
(5)	450	0.012	0.52	49.69
(6)	500	0.0011	0.52	51.78

Table 5.2 Standard value of Kappaphycus and scavenging activity

S.no	Concentration (µg/ml)	Absorbance	Blank	%RSA
(1)	250	0.105	0.52	31.8
(2)	300	0.087	0.52	35.26
(3)	350	0.066	0.52	39.3
(4)	400	0.046	0.52	43.15
(5)	450	0.027	0.52	46.8
(6)	500	0.016	0.52	48.92

Table 5.2 Standard value of gracilaria and scavenging activity

S.no	Concentration (µg/ml)	Absorbance	Blank	%RSA
(1)	250	0.102	0.52	32.57
(2)	300	0.086	0.52	35.46
(3)	350	0.063	0.52	39.88
(4)	400	0.049	0.52	42.57
(5)	450	0.031	0.52	46.02
(6)	500	0.021	0.52	47.96

In table 5.2 shows the standard values and scavenging activity of ascorbic acid, kappaphycus, gracilaria which results the %RSA of ascorbic acid is higher than other two bioactive compound

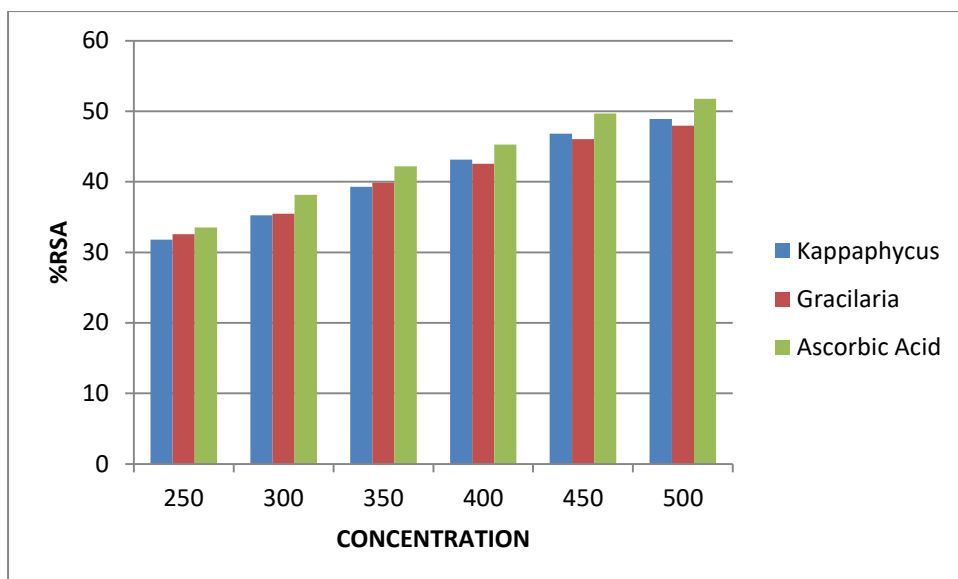


Fig 5.2.1 Comparison graph of ascorbic acid and seaweed extracts

In this fig 5.2.2 the graph explain about the standard graph of ascorbic acid concentration is higher than rest of the compound which results the kappaphycus and gracilaria are more effective than ascorbic acid the blue is kappaphyucs and the red is gracilaria and the green is standard solution ascorbic acid. The standard RSA value of ascorbic acid is start 33.53 which end to 51.78 but kappahycus start from 31.8 to 48.92 and then in gracilaria start from 32.57 to 47.96. Overall, in graph the concentration of gracilaria is lower than comparing other two solution but standard ascorbic has high concentration than other two by Li et al.,2020; Mussel inspired antioxidant activity.

5.3 ENCAPSULATION EFFICINCY :

$$\text{Encapsulation Efficiency \%} = (W_t / W_i) * 100$$

Where, Wt is the total amount of integrated material

Wi is the total amount of incorporated material added at the start of the preparation.

Result :

- The encapsulation efficiency of kappaphycus extract in liposomes is **80±0.2%**
- The encapsulation efficiency of Gracilaria extract in liposomes is **80±0.3%**

5.4 CHARATECRIZATION :

5.4.1 SEM ANALYSIS :

SEM analysis is done to lipid mixture to identify the size of liposomes in lipid mixture and their structure.

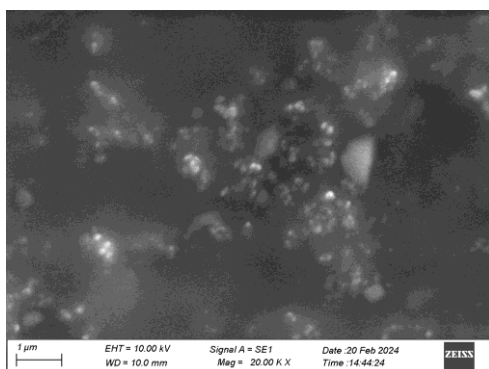


Fig 5.4.1.1 Lipid mixture

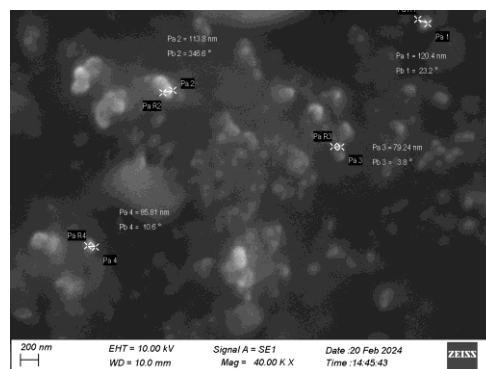


Fig 5.4.1.2 Lipid mixture in size

In this fig 5.4.1.1 and 5.4.1.2 explains the Scanning electron microscopy image which take from 1μm and 200nm meter with width of 10.0nm the fig 5.4.1.2 SEM image shows the size of liposomes in lipid mixture which is show in nano meter and the fig 5.4.1.1 shows the presence of liposomes in lipid mixture which helpful for encapsulation. Previously by Fahimirad et al.2021; liposomal SEM analysis for hydrogel formulation.

5.4.2 FTIR ANALYSIS :

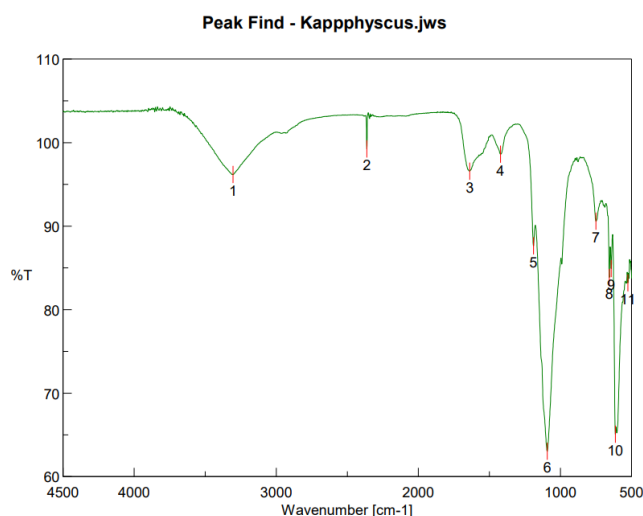


Fig 5.4.2.1 FTIR Analysis Of Kappaphycus

In this figure 5.4.2.1 Kappaphycus ftir analysis explains the peak present in powder compound. The image represents only a fraction of the spectrum, especially the wavenumber range of 4500 to 500 cm⁻¹. For a thorough study, the whole spectrum (usually 4000-400 cm⁻¹) is required. The occurrence of wide peaks across the spectrum shows that the sample is a complex combination of molecules, rather than a single pure material. While exact determination is tricky several common functional groups found in seaweed, such as hydroxyl (-OH), carbonyl (C=O), and amine (N-H), may be present based on typical absorption ranges. The peaks start from 399.193 cm⁻¹ and ends at 4500.08cm⁻¹ as shown as peak in report of Souza et al.2018; in kappaphycus.

TABLE 5.4 Kappaphycus position in Ftir graph

NO	POSITIONS	INTENSITY
1	3303.46	96.1658
2	2362.37	99.2398
3	1638.23	96.5737
4	1422.24	98.6134
5	1189.86	87.6357
6	1093.44	63.0373
7	750.174	90.5772
8	656.643	83.8422
9	643.144	84.909
10	614.217	65.0644
11	525.507	83.1919

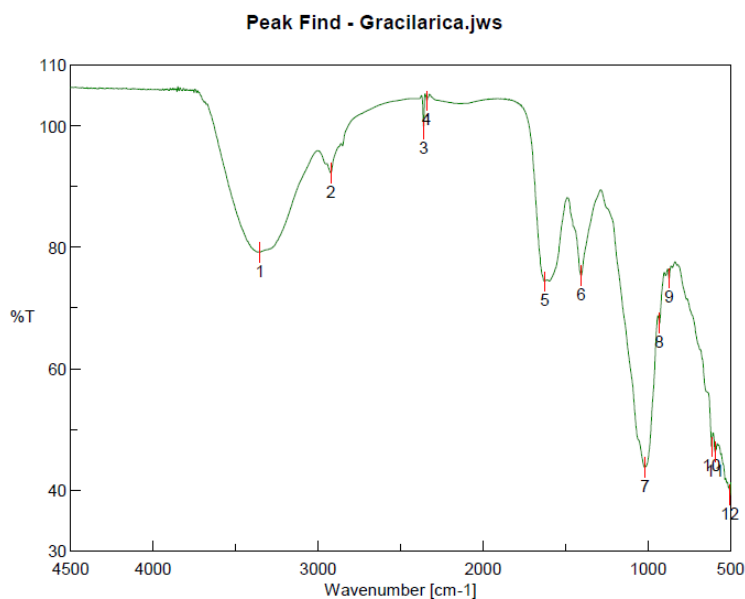


Fig 5.4.2.2 FTIR analysis of gracilaria

In this figure 5.4.2.2 Gracilaria ftir analysis explains the peak and wavenumber of powdered gracilaria compound. The picture only displays a fraction of the spectrum, especially the wavenumber range of 4500 to 500 cm⁻¹. For a thorough examination, the full spectrum spanning a larger range (usually 4000-400 cm⁻¹) is required for definite identification of functional groupings.

The appearance of wide peaks throughout the spectrum indicates that the gracilaria sample might represent a complicated combination of molecules rather than a single pure component. Specific identification is challenging in the absence of a reference spectrum; nevertheless, hydroxyl (-OH), carbonyl (C=O), and amine (N-H), three common functional groups found in seaweed, may be present based on typical absorption ranges as shown as peak in report of Sharaf and El-Naggaer 2018; in Gracilaria.

TABLE 5.4 Gracilaria positions in Ftir graph

NO	POSITIONS	INTENSITY
1	3351.68	79.1461
2	2923.56	92.2173
3	2360.44	99.4645
4	2341.16	104.067
5	1626.66	74.3535
6	1406.82	75.3082
7	1020.16	43.7246
8	931.45	67.452
9	872.631	74.8439
10	616.145	47.1473
11	594.932	46.3307

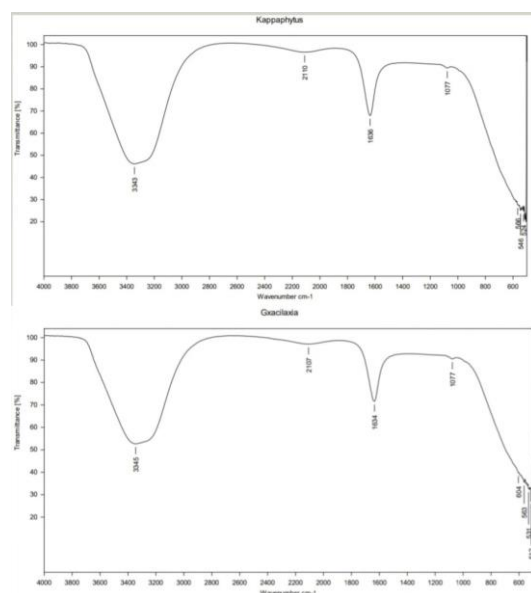


Fig 5.4.2.3 FTIR Analysis of lipid mixture K_p AND G_R

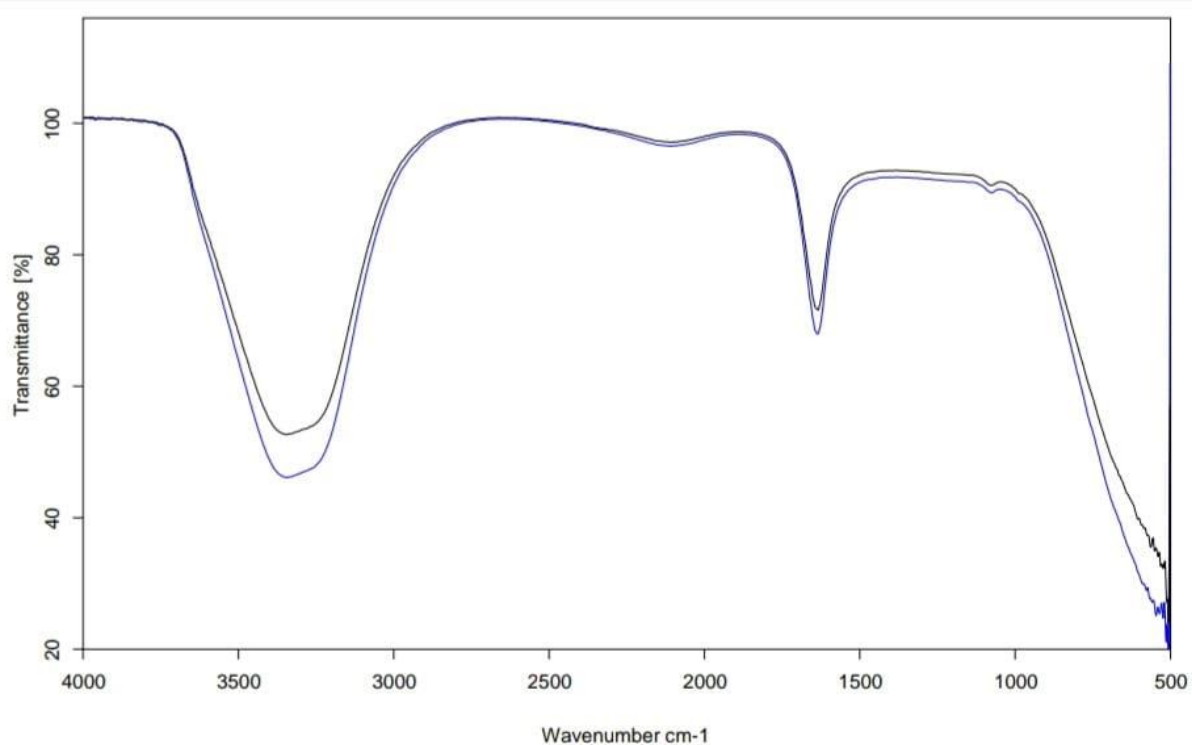


Fig 5.4.2.4 FTIR Analysis Comparing lipid mixture of K_P and G_R

5.5 VISCOSITY RESULTS :

Table 5.5 An overview of the Gellan gum gel concentration

S.no	Objectives	Temperature	GLG Concentration (g/ml)	Salt Concentration (g/ml)
(1)	Gellan gum gel concentration	25	1-3	Nil
(2)	NaCl	25	2	10
(3)	KCl	25	2	2
(4)	CaCl ₂	25	2	3

In table 5.5 explain about the gellan gum gel concentration with NaCl, KCl and CaCl₂ as which in 25 degree as shown in Sahraei and Ghaemy (2017)

5.6 GELATION TEMPERATURE :

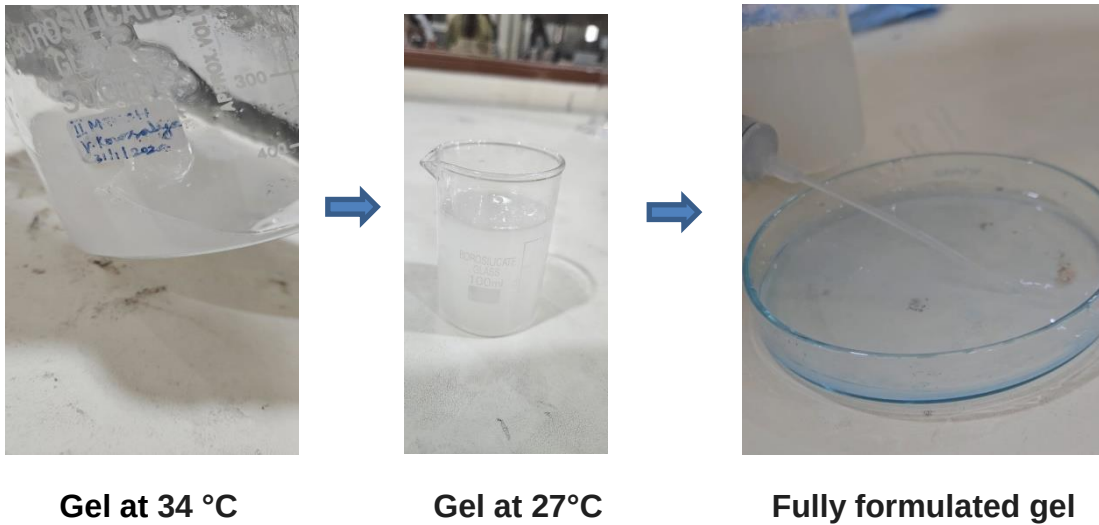


Fig 5.6 Gelation temperature

In figure 5.6.1 shows the process of gelation time and temperature where after magnetic stirring the GLG solution slightly in liquid at 34⁰c After 20 min the GLG solution become gel form at room temperature 27⁰c. Thus this is the conclusion of gelation temperature as reported done as Xing, Zheng and Duan 2015; Gellan gum gelation temperature.

5.7 BIO-INFORMATICS OF KAPPAPHYCUS AND GRACILARIA :

TABLE 5.7.1 PUBCHEM DATABASE OF PHYTOCHEMICAL COMPOUND OF KAPPAPHYCUS :

S.NO	PHYTOCHEMICAL NAME	PUBCHEM ID	SMILES
1	1-(4-Hydroxyphenethyl)isoquinoline	619372	<chem>C1=CC=C2C(=C1)C=CN=C2CCC3=CC=C(C=C3)O</chem>
2	Cholesterol	5997	<chem>CC(C)CCCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C</chem>
3	Diazoprogesterone	104633	<chem>CC12CCC3C(C1CCC2C(=O)C=[N+]=[N-])CCC4=CC(=O)CCC34C</chem>
4	1-Isothiocyanato-2,2-dimethylpropane	136393	<chem>CC(C)(C)CN=C=S</chem>
5	Oleic acid	445639	<chem>CCCCCCCCC=CCCCCCCCC(=O)O</chem>

TABLE 5.7.2 PUBCHEM DATABASE OF PHYTOCHEMICAL COMPOUND OF GRACILARIA :

S.NO	PHYTOCHEMICAL NAME	PUBCHEM ID	SMILES
1	1,2-Benzenedicarboxylic acid, mono (2-ethylhexyl)ester	20393	<chem>CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)O</chem>
2	Cholesta-8,24-dien-3-ol, 4-methyl-, (3.beta.,4.alpha.)-	22212496	<chem>CC1C2CCC3=C(C2(CCC1O)C)CCC4(C3CCC4C(C)CCC=C(C)C)C</chem>
3	N-(5-chloro-2-hydroxyphenyl)dodecanamide	536428	<chem>CCCCCCCCCCCCC(=O)NC1=CC=C(C=C1)C(=O)O</chem>
4	Folic acid	445639	<chem>CCCCCCCCC=CCCCCCCCC(=O)O</chem>
5	Pentadecanoic acid	13849	<chem>CCCCCCCCCCCCCCCCC(=O)O</chem>

5.7.3 TARGETS OF KAPPAPHYCUS :

Phytochemical	Target	Common	Uniprot ID	ChEMBL	Target Class	Probability	Known actives (3D)
1-(4-Hydroxyphenyl)	Estrogen	ESR1	P03372	CHEMBL	Nuclear receptor	0.15919	256 / 29
1-(4-Hydroxyphenyl)	Estrogen	ESR2	Q92731	CHEMBL	Nuclear receptor	0.15919	281 / 29
1-(4-Hydroxyphenyl)	Cyclin-dependent kinase	CDK2	P24941	CHEMBL	Other cytochrome	0.11204	111 / 0
1-(4-Hydroxyphenyl)	Nerve growth factor	NTRK1	P04629	CHEMBL	Kinase	0.11204	83 / 0
1-(4-Hydroxyphenyl)	Cytochrome P450	CYP17A1	P05093	CHEMBL	Cytochrome	0.11204	119 / 0
1-(4-Hydroxyphenyl)	HERG	KCNH2	Q12809	CHEMBL	Voltage-gated	0.11204	82 / 20
1-(4-Hydroxyphenyl)	Stem cell factor	KIT	P10721	CHEMBL	Kinase	0.11204	91 / 0
1-(4-Hydroxyphenyl)	Fibroblast growth factor	FGFR3	P22607	CHEMBL	Kinase	0.11204	5 / 0
1-(4-Hydroxyphenyl)	Carbonic anhydrase	CA2	P00918	CHEMBL	Lyase	0.11204	486 / 0
1-(4-Hydroxyphenyl)	Cannabinoid receptor	CNR1	P21554	CHEMBL	Family A	0.11204	170 / 0
1-(4-Hydroxyphenyl)	Carbonic anhydrase	CA1	P00915	CHEMBL	Lyase	0.11204	415 / 0
1-(4-Hydroxyphenyl)	Matrix metalloproteinase	MMP9	P14780	CHEMBL	Protease	0.11204	153 / 0
1-(4-Hydroxyphenyl)	Matrix metalloproteinase	MMP1	P03956	CHEMBL	Protease	0.11204	153 / 0
1-(4-Hydroxyphenyl)	Matrix metalloproteinase	MMP2	P08253	CHEMBL	Protease	0.11204	133 / 0
1-(4-Hydroxyphenyl)	Monoglyceride lipase	MGLL	Q99685	CHEMBL	Enzyme	0.11204	49 / 0
1-(4-Hydroxyphenyl)	Cytochrome P450	CYP11B1	P15538	CHEMBL	Cytochrome	0.11204	207 / 0
1-(4-Hydroxyphenyl)	Estradiol	HSD17B1	P14061	CHEMBL	Enzyme	0.11204	87 / 0
1-(4-Hydroxyphenyl)	Plectin	PLEC	Q15149	CHEMBL	Unclassified	0.11204	8 / 0
1-(4-Hydroxyphenyl)	Serine/threonine kinase	AKT1	P31749	CHEMBL	Kinase	0.11204	38 / 0
1-(4-Hydroxyphenyl)	Dopamine receptor	DRD5	P21918	CHEMBL	Family A	0.11204	5 / 0
1-(4-Hydroxyphenyl)	Glycogen synthase	GSK3B	P49841	CHEMBL	Kinase	0.11204	404 / 0
1-(4-Hydroxyphenyl)	Dual specific phosphatase	DUSP3	P51452	CHEMBL	Phosphatase	0.11204	19 / 0
1-(4-Hydroxyphenyl)	Carbonic anhydrase	CA6	P23280	CHEMBL	Lyase	0.11204	22 / 0
1-(4-Hydroxyphenyl)	Carbonic anhydrase	CA4	P22748	CHEMBL	Lyase	0.11204	34 / 0
1-(4-Hydroxyphenyl)	Cyclooxygenase	PTGS2	P35354	CHEMBL	Oxidoreductase	0.11204	199 / 0
1-(4-Hydroxyphenyl)	LXR-alpha	NR1H3	Q13133	CHEMBL	Nuclear receptor	0.11204	20 / 0
1-(4-Hydroxyphenyl)	Cytochrome P450	CYP3A4	P08684	CHEMBL	Cytochrome	0.11204	13 / 0
1-(4-Hydroxyphenyl)	Estradiol	HSD17B2	P37059	CHEMBL	Enzyme	0.11204	75 / 0
1-(4-Hydroxyphenyl)	11-beta-hydroxysteroid dehydrogenase	HSD11B1	P28845	CHEMBL	Enzyme	0.11204	401 / 0

Phytochemical	Target	Common	Uniprot ID	ChEMBL	Target Class	Probability	Known actives (3D)
1-(4-Hydroxyphenyl)	Arachidonate	ALOX12	P18054	CHEMBL	Enzyme	0.11204	20 / 0
1-(4-Hydroxyphenyl)	NADPH oxidase	NOX4	Q9NPH5	CHEMBL	Enzyme	0.11204	5 / 0
1-(4-Hydroxyphenyl)	NADPH oxidase	NOX1	Q9Y5S8	CHEMBL	Transmembrane	0.11204	1 / 0
1-(4-Hydroxyphenyl)	Aldehyde	ALDH2	P05091	CHEMBL	Oxidoreductase	0.11204	12 / 0
1-(4-Hydroxyphenyl)	Insulin-like	IGF1R	P08069	CHEMBL	Kinase	0.11204	43 / 0
1-(4-Hydroxyphenyl)	Fibroblast	FGFR1	P11362	CHEMBL	Kinase	0.11204	60 / 0
1-(4-Hydroxyphenyl)	Coagulation	F3	P13726	CHEMBL	Surface	0.11204	2 / 0
1-(4-Hydroxyphenyl)	Receptor	ERBB2	P04626	CHEMBL	Kinase	0.11204	111 / 0
1-(4-Hydroxyphenyl)	Epidermal	EGFR	P00533	CHEMBL	Kinase	0.11204	463 / 0
1-(4-Hydroxyphenyl)	Serine/threonine	AURKC	Q9UQB9	CHEMBL	Kinase	0.11204	4 / 0
1-(4-Hydroxyphenyl)	ALK tyrosine	ALK	Q9UM73	CHEMBL	Kinase	0.11204	41 / 0
1-(4-Hydroxyphenyl)	Tyrosine	PTK6	Q13882	CHEMBL	Kinase	0.11204	20 / 0
1-(4-Hydroxyphenyl)	Serine/threonine	AURKA	O14965	CHEMBL	Kinase	0.11204	190 / 0
1-(4-Hydroxyphenyl)	Vanilloid receptor	TRPV1	Q8NER1	CHEMBL	Voltage-gated	0.11204	352 / 0
1-(4-Hydroxyphenyl)	Activin receptor	ACVR1	Q04771	CHEMBL	Kinase	0.11204	1 / 0
1-(4-Hydroxyphenyl)	Dihydroorotate	DHODH	Q02127	CHEMBL	Oxidoreductase	0.11204	11 / 0
1-(4-Hydroxyphenyl)	SUMO-acyltransferase	SAE1	Q9UBE0	CHEMBL	Enzyme	0.11204	7 / 0
1-(4-Hydroxyphenyl)	Testis-specific	SHBG	P04278	CHEMBL	Secreted	0.11204	12 / 0
1-(4-Hydroxyphenyl)	Cyclin-dependent	CCNE2	O96020	CHEMBL	Other cytoplasmic	0.11204	48 / 0
1-(4-Hydroxyphenyl)	Cyclin-dependent	CCNB3	Q8WWL7	CHEMBL	Other cytoplasmic	0.11204	85 / 0
1-(4-Hydroxyphenyl)	Glycogen	GSK3A	P49840	CHEMBL	Kinase	0.11204	39 / 0
1-(4-Hydroxyphenyl)	Cyclin-dependent	CDK5	Q00535	CHEMBL	Kinase	0.11204	14 / 0
1-(4-Hydroxyphenyl)	Cystic fibrosis	CFTR	P13569	CHEMBL	Other ion channel	0.11204	2 / 0
1-(4-Hydroxyphenyl)	Hepatocyte	MET	P08581	CHEMBL	Kinase	0.11204	277 / 0
1-(4-Hydroxyphenyl)	Epoxide hydrolase	EPHX1	P07099	CHEMBL	Protease	0.11204	30 / 0
1-(4-Hydroxyphenyl)	Kinesin-1	RET	P07949	CHEMBL	Kinase	0.11204	47 / 0
1-(4-Hydroxyphenyl)	Tubulin binding	TUBB1	Q9H4B7	CHEMBL	Structural	0.11204	10 / 0
1-(4-Hydroxyphenyl)	Potassium	ATP4B	P51164	CHEMBL	Primary active	0.11204	37 / 0
1-(4-Hydroxyphenyl)	3-phosphoinositide	PDPK1	O15530	CHEMBL	Kinase	0.11204	36 / 0

Phytochemical	Target	Common	Uniprot ID	ChEMBL	Target Class	Probability	Known actives (3D)
Cholesterol	Cytochrome	CYP51A1	Q16850	CHEMBL	Cytochrome	0.63227	3 / 2Â Â Â Â Â
Cholesterol	HMG-CoA	HMGCR	P04035	CHEMBL	Oxidoreductase	0.63227	74 / 7Â Â Â Â Â
Cholesterol	Cytochrome	CYP17A1	P05093	CHEMBL	Cytochrome	0.62401	53 / 50Â Â Â Â Â
Cholesterol	Androgen	AR	P10275	CHEMBL	Nuclear receptor	0.59949	56 / 102Â Â Â Â Â
Cholesterol	Estrogen	ESR2	Q92731	CHEMBL	Nuclear receptor	0.58301	14 / 47Â Â Â Â Â
Cholesterol	Estrogen	ESR1	P03372	CHEMBL	Nuclear receptor	0.50109	16 / 39Â Â Â Â Â
Cholesterol	Testis-specific	SHBG	P04278	CHEMBL	Secreted	0.50109	6 / 48Â Â Â Â Â
Cholesterol	LXR-alpha	NR1H3	Q13133	CHEMBL	Nuclear receptor	0.50109	16 / 20Â Â Â Â Â
Cholesterol	Niemann-Pick	NPC1L1	Q9UHC9	CHEMBL	Other membrane	0.45183	4 / 13Â Â Â Â Â
Cholesterol	Sterol regulatory	SREBF2	Q12772	CHEMBL	Unclassified	0.45183	0 / 1Â Â Â Â Â
Cholesterol	Cytochrome	CYP19A1	P11511	CHEMBL	Cytochrome	0.44368	22 / 161Â Â Â Â Â
Cholesterol	Nuclear receptor	RORC	P51449	CHEMBL	Nuclear receptor	0.37804	7 / 9Â Â Â Â Â
Cholesterol	Serotonin	SLC6A4	P31645	CHEMBL	Electrotransporter	0.14853	15 / 5Â Â Â Â Â
Cholesterol	Norepinephrine	SLC6A2	P23975	CHEMBL	Electrotransporter	0.12394	5 / 2Â Â Â Â Â
Cholesterol	Muscarinic	CHRM2	P08172	CHEMBL	Family A	0.12394	5 / 1Â Â Â Â Â
Cholesterol	Acetylcholine	ACHE	P22303	CHEMBL	Hydrolase	0.12394	3 / 1Â Â Â Â Â
Cholesterol	Cytochrome	CYP2C19	P33261	CHEMBL	Cytochrome	0.12394	6 / 3Â Â Â Â Â
Cholesterol	Protein-tyrosine	PTPN1	P18031	CHEMBL	Phosphatase	0.12394	16 / 47Â Â Â Â Â
Cholesterol	Butyrylcholinesterase	BCHE	P06276	CHEMBL	Hydrolase	0.11574	4 / 2Â Â Â Â Â
Cholesterol	Glucose-6-phosphate	G6PD	P11413	CHEMBL	Enzyme	0.11574	4 / 2Â Â Â Â Â
Cholesterol	Corticosteroid	SERPINA	P08185	CHEMBL	Secreted	0.11574	2 / 18Â Â Â Â Â
Cholesterol	Nuclear receptor	RORA	P35398	CHEMBL	Nuclear receptor	0.11574	1 / 3Â Â Â Â Â
Cholesterol	Dual specific	CDC25A	P30304	CHEMBL	Phosphatase	0.11574	5 / 11Â Â Â Â Â
Cholesterol	Vitamin D	VDNR	P11473	CHEMBL	Nuclear receptor	0.11574	7 / 49Â Â Â Â Â
Cholesterol	Prostanoid	PTGER1	P34995	CHEMBL	Family A	0.11574	0 / 9Â Â Â Â Â
Cholesterol	Prostanoid	PTGER2	P43116	CHEMBL	Family A	0.11574	0 / 20Â Â Â Â Â
Cholesterol	LXR-beta	NR1H2	P55055	CHEMBL	Nuclear receptor	0.11574	8 / 1Â Â Â Â Â
Cholesterol	11-beta-hydroxysteroid	HSD11B1	P28845	CHEMBL	Enzyme	0.11574	136 / 23Â Â Â Â Â
Cholesterol	Nuclear receptor	NR1I3	Q14994	CHEMBL	Nuclear receptor	0.11574	2 / 3Â Â Â Â Â
Cholesterol	Carboxylesterase	CES2	O00748	CHEMBL	Enzyme	0.11574	4 / 10Â Â Â Â Â
Cholesterol	Glucocorticoid	NR3C1	P04150	CHEMBL	Nuclear receptor	0.11574	50 / 25Â Â Â Â Â
Cholesterol	Peroxisome	PPARA	Q07869	CHEMBL	Nuclear receptor	0.11574	0 / 11Â Â Â Â Â
Cholesterol	Peroxisome	PPARD	Q03181	CHEMBL	Nuclear receptor	0.11574	0 / 8Â Â Â Â Â
Cholesterol	Squalene	SQLE	Q14534	CHEMBL	Enzyme	0.11574	0 / 4Â Â Â Â Â
Cholesterol	T-cell protein	PTPN2	P17706	CHEMBL	Phosphatase	0.11574	1 / 15Â Â Â Â Â
Cholesterol	Glycine receptor	GLRA1	P23415	CHEMBL	Ligand-gated	0.11574	1 / 1Â Â Â Â Â
Cholesterol	Thromboxane	TBXAS1	P24557	CHEMBL	Cytochrome	0.11574	3 / 1Â Â Â Â Â
Cholesterol	Protein-tyrosine	PTPN6	P29350	CHEMBL	Phosphatase	0.11574	0 / 1Â Â Â Â Â
Cholesterol	C-C chemokine	CCR1	P32246	CHEMBL	Family A	0.11574	74 / 0Â Â Â Â Â
Cholesterol	Dual specific	CDC25B	P30305	CHEMBL	Phosphatase	0.11574	5 / 7Â Â Â Â Â
Cholesterol	Prostaglandin	PTGES	O14684	CHEMBL	Enzyme	0.11574	6 / 10Â Â Â Â Â
Cholesterol	Sigma opiate	SIGMAR1	Q99720	CHEMBL	Membrane	0.11574	16 / 5Â Â Â Â Â
Cholesterol	Serotonin	HTR2B	P41595	CHEMBL	Family A	0.11574	4 / 0Â Â Â Â Â
Cholesterol	Adrenergic	ADRA2C	P18825	CHEMBL	Family A	0.11574	1 / 0Â Â Â Â Â
Cholesterol	Sonic hedgehog	SHH	Q15465	CHEMBL	Unclassified	0.11574	0 / 1Â Â Â Â Â
Cholesterol	Peroxisome	PPARG	P37231	CHEMBL	Nuclear receptor	0.11574	0 / 12Â Â Â Â Â
Cholesterol	Protein kinase	PRKCG	P05129	CHEMBL	Kinase	0.11574	8 / 0Â Â Â Â Â
Cholesterol	Protein kinase	PRKCD	Q05655	CHEMBL	Kinase	0.11574	19 / 0Â Â Â Â Â
Cholesterol	Protein kinase	PRKCB	P05771	CHEMBL	Kinase	0.11574	7 / 0Â Â Â Â Â
Cholesterol	Protein kinase	PRKCE	Q02156	CHEMBL	Kinase	0.11574	9 / 0Â Â Â Â Â

Phytochemical	Target	Common Name	Uniprot ID	ChEMBL ID	Target Class	Probability	Known actives (3D)
Cholesterol	Protein kinase	PRKCQ	Q04759	CHEMBL	Kinase	0.11574	7 / 0
Cholesterol	Dopamine	DRD2	P14416	CHEMBL	Family A	0.11574	22 / 0
Cholesterol	11-beta-hydroxysteroid	HSD11B2	P80365	CHEMBL	Enzyme	0.11574	11 / 8
Cholesterol	DNA polymerase	POLB	P06746	CHEMBL	Enzyme	0.11574	0 / 6
Cholesterol	Anti-estrogen	DHCR7	Q9UBM7	CHEMBL	Enzyme	0.11574	2 / 5
Cholesterol	Prolyl endopeptidase	PREP	P48147	CHEMBL	Protease	0.11574	0 / 1
Diazopropane	Mineralocorticoid	NR3C2	P08235	CHEMBL	Nuclear receptor	0.09724	12 / 21
Diazopropane	Androgen	AR	P10275	CHEMBL	Nuclear receptor	0.09724	0 / 54
Diazopropane	Corticosteroid	SERPINA1	P08185	CHEMBL	Secreted	0.09724	0 / 18
Diazopropane	Sigma opiate	SIGMAR1	Q99720	CHEMBL	Membrane	0.09724	0 / 2
Diazopropane	Testis-specific	SHBG	P04278	CHEMBL	Secreted	0.09724	0 / 30
Diazopropane	Pregnane	NR1I2	O75469	CHEMBL	Nuclear receptor	0.09724	0 / 2
Diazopropane	Estradiol	HSD17B3	P37058	CHEMBL	Enzyme	0.09724	0 / 1
Diazopropane	Fatty acid	FABP1	P07148	CHEMBL	Fatty acid	0.09724	0 / 3
Diazopropane	Steroid 5-alpha	SRD5A1	P18405	CHEMBL	Oxidoreductase	0.09724	5 / 7
Diazopropane	Steroid 5-alpha	SRD5A2	P31213	CHEMBL	Oxidoreductase	0.09724	5 / 12
Diazopropane	Cytochrome	CYP17A1	P05093	CHEMBL	Cytochrome	0.09724	6 / 20
Diazopropane	Nuclear receptor	NR1I3	Q14994	CHEMBL	Nuclear receptor	0.09724	0 / 1
Diazopropane	Cytochrome	CYP19A1	P11511	CHEMBL	Cytochrome	0.09724	4 / 240
Diazopropane	Niemann-Pick	NPC1L1	Q9UHC9	CHEMBL	Other membrane	0.09724	0 / 3
1-Isothiocyanate	Transient receptor	TRPA1	O75762	CHEMBL	Voltage-gated	0.61203	13 / 11
Oleic acid	Fatty acid	FABP4	P15090	CHEMBL	Fatty acid	0.11574	15 / 4
Oleic acid	Anandamide	FAAH	O00519	CHEMBL	Enzyme	0.11574	16 / 17
Oleic acid	Peroxisome	PPARG	P37231	CHEMBL	Nuclear receptor	0.11574	240 / 24
Oleic acid	Peroxisome	PPARA	Q07869	CHEMBL	Nuclear receptor	0.11574	174 / 19
Oleic acid	Telomerase	TERT	O14746	CHEMBL	Enzyme	0.11574	11 / 2
Oleic acid	Fatty acid	FABP5	Q01469	CHEMBL	Fatty acid	0.11574	12 / 2
Oleic acid	Peroxisome	PPARD	Q03181	CHEMBL	Nuclear receptor	0.11574	160 / 12
Oleic acid	Fatty acid	FABP1	P07148	CHEMBL	Fatty acid	0.11574	11 / 3

Phytochemical	Target	Common Name	Uniprot ID	ChEMBL ID	Target Class	Probability	Known actives (3D)
Oleic acid	11-beta-hydroxylase	HSD11B1	P28845	CHEMBL1211	Enzyme	0.10877	27 / 42
Oleic acid	Cytochrome P450 19A1	CYP19A1	P11511	CHEMBL1211	Cytochrome P450	0.10877	0 / 259
Oleic acid	CD81 antigen	CD81	P60033	CHEMBL1211	Surface antigen	0.10058	0 / 1
Oleic acid	Protein kinase C	PRKCH	P24723	CHEMBL1211	Kinase	0.10058	0 / 1
Oleic acid	LXR-alpha	NR1H3	Q13133	CHEMBL1211	Nuclear receptor	0.10058	6 / 20
Oleic acid	Cyclooxygenase	PTGS2	P35354	CHEMBL1211	Oxidoreductase	0.10058	11 / 4
Oleic acid	Dual specific tyrosine phosphatase	CDC25A	P30304	CHEMBL1211	Phosphatase	0.10058	16 / 16
Oleic acid	Corticosteroid 11-beta-dehydrogenase	SERPINA1	P08185	CHEMBL1211	Secreted protein	0.10058	0 / 23
Oleic acid	Testis-specific protein	SHBG	P04278	CHEMBL1211	Secreted protein	0.10058	0 / 55
Oleic acid	Glucose-6-phosphate dehydrogenase	G6PD	P11413	CHEMBL1211	Enzyme	0.10058	0 / 7
Oleic acid	Cytochrome P450 51A1	CYP51A1	Q16850	CHEMBL1211	Cytochrome P450	0.10058	0 / 2
Oleic acid	Carboxylesterase	CES2	O00748	CHEMBL1211	Enzyme	0.10058	1 / 14
Oleic acid	DNA polymerase	POLB	P06746	CHEMBL1211	Enzyme	0.10058	1 / 8
Oleic acid	Receptor tyrosine kinase	PTPRF	P10586	CHEMBL1211	Membrane protein	0.10058	15 / 1
Oleic acid	Protein tyrosine phosphatase	PTPN11	Q06124	CHEMBL1211	Phosphatase	0.10058	16 / 2
Oleic acid	Vanilloid receptor	TRPV1	Q8NER1	CHEMBL1211	Voltage-gated ion channel	0.10058	0 / 4
Oleic acid	Glucocorticoid receptor	NR3C1	P04150	CHEMBL1211	Nuclear receptor	0.10058	28 / 36
Oleic acid	Protein farnesyl transferase	FNTA	P49354	CHEMBL1211	Enzyme	0.10058	15 / 14
Oleic acid	Niemann-Pick C1-like 1	NPC1L1	Q9UHC9	CHEMBL1211	Other membrane protein	0.10058	0 / 11
Oleic acid	Sigma opioid receptor	SIGMAR1	Q99720	CHEMBL1211	Membrane protein	0.10058	0 / 4
Oleic acid	Cytochrome P450 17A1	CYP17A1	P05093	CHEMBL1211	Cytochrome P450	0.10058	0 / 43
Oleic acid	Low molecular weight tyrosine phosphatase	ACP1	P24666	CHEMBL1211	Phosphatase	0.10058	15 / 1
Oleic acid	Prostanoid synthase	PTGIR	P43119	CHEMBL1211	Family A	0.10058	94 / 8
Oleic acid	Androgen receptor	AR	P10275	CHEMBL1211	Nuclear receptor	0.10058	1 / 126
Oleic acid	Phospholipase A2 group I	PLA2G1E	P04054	CHEMBL1211	Enzyme	0.10058	1 / 1
Oleic acid	Dopamine transporter	SLC6A3	Q01959	CHEMBL1211	Electrochemical transporter	0.10058	0 / 1
Oleic acid	Adenosine deaminase	ADORA3	P0DMS8	CHEMBL1211	Family A	0.10058	0 / 3
Oleic acid	MAP kinase	MAPK3	P27361	CHEMBL1211	Kinase	0.10058	0 / 1
Oleic acid	Prostanoid synthase	PTGER1	P34995	CHEMBL1211	Family A	0.10058	20 / 12
Oleic acid	Butyrylcholinesterase	BCHE	P06276	CHEMBL1211	Hydrolase	0.10058	0 / 2
Oleic acid	Beta-secretase	BACE1	P56817	CHEMBL1211	Protease	0.10058	0 / 2
Oleic acid	Nuclear receptor	NR1I3	Q14994	CHEMBL1211	Nuclear receptor	0.10058	0 / 2
Oleic acid	DNA topoisomerase	TOP2A	P11388	CHEMBL1211	Isomerase	0.10058	0 / 2

5.7.4 TABLE OF TARGETS FOR GRACILARIA :

Phytochemical	Target	Common	Uniprot ID	ChEMBL	Target Class	Probability	Known active
1,2- Benz	T-cell protein	PTPN2	P17706	CHEMBL	Phosphatase	0.10058	20 / 7
1,2- Benz	G protein-coupled	PTGDR2	Q9Y5Y4	CHEMBL	Family A	0.10058	1095 / 0
1,2- Benz	Prostanoid	PTGER1	P34995	CHEMBL	Family A	0.10058	340 / 0
1,2- Benz	Induced nuclear	MCL1	Q07820	CHEMBL	Other cytochrome	0.10058	81 / 0
1,2- Benz	p53-binding	MDM2	Q00987	CHEMBL	Other nuclear	0.10058	156 / 0
1,2- Benz	Solute carrier	SLC22A6	Q4U2R8	CHEMBL	Electrotransporter	0.10058	3 / 0
1,2- Benz	Protein kinase	PRKCD	Q05655	CHEMBL	Kinase	0.10058	0 / 8
1,2- Benz	Casein kinase	CSNK2A1	P68400	CHEMBL	Kinase	0.10058	107 / 0
1,2- Benz	Aldo-keto reductase	AKR1C3	P42330	CHEMBL	Enzyme	0.10058	156 / 0
1,2- Benz	Aldo-keto reductase	AKR1C1	Q04828	CHEMBL	Enzyme	0.10058	12 / 0
1,2- Benz	Gamma-glutamyl	ABAT	P80404	CHEMBL	Transferase	0.10058	4 / 0
1,2- Benz	Protein-tyrosine	PTPN1	P18031	CHEMBL	Phosphatase	0.10058	59 / 10
1,2- Benz	Leukotrien synthase	LTB4R	Q15722	CHEMBL	Family A	0.10058	55 / 0
1,2- Benz	Solute carrier	SLC22A1	Q96S37	CHEMBL	Electrotransporter	0.10058	72 / 0
1,2- Benz	Plasma retinol	RBP4	P02753	CHEMBL	Secreted	0.10058	19 / 0
1,2- Benz	5-lipoxygenase	ALOX5A	P20292	CHEMBL	Other cytochrome	0.10058	78 / 0
1,2- Benz	Angiotensin	ACE	P12821	CHEMBL	Protease	0.10058	355 / 0
1,2- Benz	MAP kinase	MAPK14	Q16539	CHEMBL	Kinase	0.10058	35 / 0
1,2- Benz	MAP kinase	MAPK1	P28482	CHEMBL	Kinase	0.10058	6 / 0
1,2- Benz	Monocarboxylate	SLC16A1	P53985	CHEMBL	Electrotransporter	0.10058	23 / 0
1,2- Benz	Apoptosis	BCL2	P10415	CHEMBL	Other ion channel	0.10058	34 / 0
1,2- Benz	Retinoic acid	RARG	P13631	CHEMBL	Nuclear receptor	0.10058	48 / 0
1,2- Benz	Thromboxane synthase	TBXS1	P24557	CHEMBL	Cytochrome	0.10058	283 / 0
1,2- Benz	Aldose reductase	AKR1B1	P15121	CHEMBL	Enzyme	0.10058	348 / 0
1,2- Benz	Fatty acid	FABP4	P15090	CHEMBL	Fatty acid	0.10058	79 / 0
1,2- Benz	Matrix metalloproteinase	MMP13	P45452	CHEMBL	Protease	0.10058	77 / 0
1,2- Benz	Matrix metalloproteinase	MMP9	P14780	CHEMBL	Protease	0.10058	79 / 0
1,2- Benz	Matrix metalloproteinase	MMP2	P08253	CHEMBL	Protease	0.10058	151 / 0
1,2- Benz	Matrix metalloproteinase	MMP8	P22894	CHEMBL	Protease	0.10058	88 / 0
1,2- Benz	Apoptosis	BCL2L1	Q07817	CHEMBL	Other ion channel	0.10058	37 / 0
1,2- Benz	Aldo-keto reductase	AKR1C2	P52895	CHEMBL	Enzyme	0.10058	44 / 0
1,2- Benz	Retinoid	RXR	P28702	CHEMBL	Nuclear receptor	0.10058	62 / 0
1,2- Benz	Dihydroxy	DHODH	Q02127	CHEMBL	Oxidoreductase	0.10058	172 / 0
1,2- Benz	Retinoid	RXR	P48443	CHEMBL	Nuclear receptor	0.10058	108 / 0
1,2- Benz	Prostanoid	PTGER2	P43116	CHEMBL	Family A	0.10058	110 / 0
1,2- Benz	Cyclooxygenase	PTGS2	P35354	CHEMBL	Oxidoreductase	0.10058	147 / 0
1,2- Benz	Prostanoid	PTGDR	Q13258	CHEMBL	Family A	0.10058	172 / 0
1,2- Benz	C-C chemokine	CCR9	P51686	CHEMBL	Family A	0.10058	17 / 0
1,2- Benz	Androgen	AR	P10275	CHEMBL	Nuclear receptor	0.10058	12 / 1

Phytochemical	Target	Common	Uniprot ID	ChEMBL	Target Class	Probability	Known actives (3D)
1,2- Benz	C-C chem	CCR2	P41597	CHEMBL	Family A	0.10058	51 / 0
1,2- Benz	Angiotens	AGTR2	P50052	CHEMBL	Family A	0.10058	13 / 0
1,2- Benz	Steroid 5-	SRD5A2	P31213	CHEMBL	Oxidoreductase	0.10058	35 / 0
1,2- Benz	Type-1 ar	AGTR1	P30556	CHEMBL	Family A	0.10058	130 / 0
1,2- Benz	Autotaxin	ENPP2	Q13822	CHEMBL	Enzyme	0.10058	18 / 0
1,2- Benz	Transthyrin	TTR	P02766	CHEMBL	Secreted	0.10058	8 / 0
1,2- Benz	Free fatty	FFAR1	O14842	CHEMBL	Family A	0.10058	134 / 0
1,2- Benz	Fatty acid	FABP1	P07148	CHEMBL	Fatty acid	0.10058	6 / 0
1,2- Benz	Thromboxan	TBXA2R	P21731	CHEMBL	Family A	0.10058	275 / 0
1,2- Benz	Aldehyde	AKR1A1	P14550	CHEMBL	Enzyme	0.10058	19 / 0
1,2- Benz	Lysine-sp	KDM5A	P29375	CHEMBL	Eraser	0.10058	8 / 0
1,2- Benz	Cholecyst	CCKBR	P32239	CHEMBL	Family A	0.10058	89 / 0
1,2- Benz	Prostanoid	PTGER3	P43115	CHEMBL	Family A	0.10058	49 / 0
1,2- Benz	Lysine-sp	KDM5B	Q9UGL1	CHEMBL	Eraser	0.10058	7 / 0
1,2- Benz	Lysine-sp	KDM2B	Q8NHM5	CHEMBL	Eraser	0.10058	3 / 0
1,2- Benz	Aldo-keto	AKR1B10	O60218	CHEMBL	Enzyme	0.10058	18 / 0
1,2- Benz	Prostanoid	PTGER4	P35408	CHEMBL	Family A	0.10058	129 / 0
1,2- Benz	Matrix metallo	MMP3	P08254	CHEMBL	Protease	0.10058	91 / 0
1,2- Benz	Hematopoietic	PTPN22	Q9Y2R2	CHEMBL	Phosphatase	0.10058	7 / 0
1,2- Benz	Matrix metallo	MMP1	P03956	CHEMBL	Protease	0.10058	45 / 0
1,2- Benz	G-protein	FFAR4	Q5NUL3	CHEMBL	Family A	0.10058	20 / 0
1,2- Benz	Cyclooxygenase	PTGS1	P23219	CHEMBL	Oxidoreductase	0.10058	50 / 0
1,2- Benz	Neprilysin	MME	P08473	CHEMBL	Protease	0.10058	249 / 0
1,2- Benz	Endothelin	ECE1	P42892	CHEMBL	Protease	0.10058	80 / 0
1,2- Benz	Hepatocyte	HNF4A	P41235	CHEMBL	Unclassified	0.10058	11 / 0
1,2- Benz	Lysine-sp	KDM2A	Q9Y2K7	CHEMBL	Eraser	0.10058	16 / 0
1,2- Benz	Lysine-sp	KDM5C	P41229	CHEMBL	Eraser	0.10058	22 / 0
1,2- Benz	Methionyl	MARS	P56192	CHEMBL	Enzyme	0.10058	14 / 0
1,2- Benz	Chymase	CMA1	P23946	CHEMBL	Protease	0.10058	101 / 0
1,2- Benz	Steroid 5-	SRD5A1	P18405	CHEMBL	Oxidoreductase	0.10058	8 / 0
1,2- Benz	L-lactate dehydrogenase	LDHA	P00338	CHEMBL	Enzyme	0.10058	44 / 0
1,2- Benz	L-lactate dehydrogenase	LDHB	P07195	CHEMBL	Enzyme	0.10058	16 / 0
1,2- Benz	Transitional	VCP	P55072	CHEMBL	Primary amine	0.10058	14 / 0
1,2- Benz	DNA topoisomerase	TOP1	P11387	CHEMBL	Isomerase	0.10058	2 / 0
1,2- Benz	Thyroid hormone	THRA	P10827	CHEMBL	Nuclear receptor	0.10058	25 / 0
1,2- Benz	Thyroid hormone	THRB	P10828	CHEMBL	Nuclear receptor	0.10058	30 / 0
1,2- Benz	Endothelin	EDNRA	P25101	CHEMBL	Family A	0.10058	202 / 0
1,2- Benz	Vitronectin	ITGAV	P06756	CHEMBL	Membrane	0.10058	30 / 0
1,2- Benz	Cathepsin	CTSG	P08311	CHEMBL	Protease	0.10058	12 / 0
1,2- Benz	Phosphodiesterase	PDE10A	Q9Y233	CHEMBL	Phosphodiesterase	0.10058	10 / 0

Phytochemical	Target	Common	Uniprot ID	ChEMBL	Target Class	Probability	Known actives (3D)
1,2- Benz	Aldo-keto	AKR1C4	P17516	CHEMBL	Enzyme	0.10058	4 / 0
1,2- Benz	c-Jun N-ter	MAPK8	P45983	CHEMBL	Kinase	0.10058	27 / 0
1,2- Benz	Lysosomal	CTSA	P10619	CHEMBL	Protease	0.10058	327 / 0
1,2- Benz	Integrin al	ITGB1 IT	P05556	CHEMBL	Unclassifi	0.10058	30 / 0
1,2- Benz	Histone d	HDAC3	O15379	CHEMBL	Eraser	0.10058	1 / 0
1,2- Benz	Histone d	HDAC6	Q9UBN7	CHEMBL	Eraser	0.10058	2 / 0
1,2- Benz	Histone d	HDAC2	Q92769	CHEMBL	Eraser	0.10058	1 / 0
1,2- Benz	Histone d	HDAC8	Q9BY41	CHEMBL	Eraser	0.10058	1 / 0
1,2- Benz	Histone d	HDAC1	Q13547	CHEMBL	Eraser	0.10058	4 / 0
1,2- Benz	Histone d	HDAC10	Q969S8	CHEMBL	Eraser	0.10058	1 / 0
1,2- Benz	Transient	TRPM8	Q7Z2W7	CHEMBL	Voltage-g	0.10058	64 / 0
1,2- Benz	ADAMTS	ADAMTS	O75173	CHEMBL	Protease	0.10058	8 / 0
1,2- Benz	3-phosph	PDPK1	O15530	CHEMBL	Kinase	0.10058	3 / 0
1,2- Benz	Mitogen-e	MAP3K8	P41279	CHEMBL	Kinase	0.10058	10 / 0
1,2- Benz	6-phosph	PFKFB3	Q16875	CHEMBL	Enzyme	0.10058	14 / 0
1,2- Benz	Fatty acid	FABP3	P05413	CHEMBL	Fatty acid	0.10058	31 / 0
1,2- Benz	Fatty acid	FABP5	Q01469	CHEMBL	Fatty acid	0.10058	11 / 0
1,2- Benz	Interleukin	CXCL8	P10145	CHEMBL	Secreted	0.10058	12 / 0
1,2- Benz	AMP dea	AMPD3	Q01432	CHEMBL	Enzyme	0.10058	1 / 0
1,2- Benz	Axin1/beta	CTNNB1	P35222	CHEMBL	Unclassifi	0.10058	1 / 0
1,2- Benz	Inosine-5'	IMPDH2	P12268	CHEMBL	Oxidoredu	0.10058	18 / 0
Cholesta	Androgen	AR	P10275	CHEMBL	Nuclear re	0.46415	18 / 106
Cholesta	Norepine	SLC6A2	P23975	CHEMBL	Electroch	0.37641	2 / 2
Cholesta	HMG-CoA	HMGCR	P04035	CHEMBL	Oxidoredu	0.33256	40 / 22
Cholesta	Cytochro	CYP51A1	Q16850	CHEMBL	Cytochro	0.33256	3 / 2
Cholesta	LXR-alpha	NR1H3	Q13133	CHEMBL	Nuclear re	0.25355	15 / 20
Cholesta	Butyrylch	BCHE	P06276	CHEMBL	Hydrolase	0.23605	6 / 2
Cholesta	Niemann	NPC1L1	Q9UHC9	CHEMBL	Other me	0.20971	9 / 13
Cholesta	Nuclear re	RORC	P51449	CHEMBL	Nuclear re	0.1921	7 / 9
Cholesta	Protein-ty	PTPN1	P18031	CHEMBL	Phosphat	0.1834	14 / 52
Cholesta	Cytochro	CYP17A1	P05093	CHEMBL	Cytochro	0.1834	25 / 51
Cholesta	Estrogen	ESR1	P03372	CHEMBL	Nuclear re	0.16584	7 / 40
Cholesta	Serotonin	SLC6A4	P31645	CHEMBL	Electroch	0.16584	3 / 5
Cholesta	Acetylcho	ACHE	P22303	CHEMBL	Hydrolase	0.14831	6 / 1
Cholesta	Sterol reg	SREBF2	Q12772	CHEMBL	Unclassifi	0.14831	0 / 1
Cholesta	Cytochro	CYP19A1	P11511	CHEMBL	Cytochro	0.14831	2 / 190
Cholesta	Cytochro	CYP2C19	P33261	CHEMBL	Cytochro	0.12199	2 / 3
Cholesta	Muscarini	CHRM2	P08172	CHEMBL	Family A	0.11321	1 / 2
Cholesta	Nuclear re	NR1I3	Q14994	CHEMBL	Nuclear re	0.10444	0 / 3
Cholesta	Testis-sp	SHBG	P04278	CHEMBL	Secreted	0.10444	1 / 48

Phytochemical	Target	Common	Uniprot ID	ChEMBL	Target Class	Probability	Known actives (3D)
Cholesterol	Estrogen	ESR2	Q92731	CHEMBL	Nuclear receptor	0.09566	5 / 48
N-(5-chloro)	Epoxide hydrolase	EPHX2	P34913	CHEMBL	Protease	0.1115	57 / 49
N-(5-chloro)	Kinesin-1	RET	P07949	CHEMBL	Kinase	0.1115	19 / 0
N-(5-chloro)	P2X purin	P2RX7	Q99572	CHEMBL	Ligand-gated	0.1115	4 / 4
N-(5-chloro)	Arachidonic acid	ALOX5	P09917	CHEMBL	Oxidoreductase	0.1115	144 / 0
N-(5-chloro)	Macrophage	MPEG1	Q2M385	CHEMBL	Unclassified	0.1115	12 / 0
N-(5-chloro)	Acyl-CoA	SCD	O00767	CHEMBL	Enzyme	0.1115	13 / 0
N-(5-chloro)	Apoptosis	BCL2L1	Q07817	CHEMBL	Other ion channel	0.1115	14 / 0
N-(5-chloro)	Cannabinoid	CNR2	P34972	CHEMBL	Family A	0.1115	88 / 23
N-(5-chloro)	Serine/threonine	WEE1	P30291	CHEMBL	Kinase	0.1115	72 / 0
N-(5-chloro)	Tyrosine	SRC	P12931	CHEMBL	Kinase	0.1115	64 / 0
N-(5-chloro)	Cannabinoid	CNR1	P21554	CHEMBL	Family A	0.1115	115 / 15
N-(5-chloro)	Aldose reductase	AKR1B1	P15121	CHEMBL	Enzyme	0.1115	30 / 0
N-(5-chloro)	Estradiol	HSD17B1	P14061	CHEMBL	Enzyme	0.1115	158 / 0
N-(5-chloro)	Cytochrome	CYP2C9	P11712	CHEMBL	Cytochrome	0.1115	6 / 0
N-(5-chloro)	Cytochrome	CYP3A4	P08684	CHEMBL	Cytochrome	0.1115	5 / 0
N-(5-chloro)	Cytochrome	CYP2C19	P33261	CHEMBL	Cytochrome	0.1115	6 / 0
N-(5-chloro)	Alpha-ketoglutarate	FTO	Q9C0B1	CHEMBL	Oxidoreductase	0.1115	0 / 1
N-(5-chloro)	Histone deacetylase	HDAC6	Q9UBN7	CHEMBL	Eraser	0.1115	146 / 68
N-(5-chloro)	Histone deacetylase	HDAC2	Q92769	CHEMBL	Eraser	0.1115	80 / 48
N-(5-chloro)	Histone deacetylase	HDAC8	Q9BY41	CHEMBL	Eraser	0.1115	123 / 51
N-(5-chloro)	Monoamine oxidase	MAOA	P21397	CHEMBL	Oxidoreductase	0.1115	25 / 0
N-(5-chloro)	11-beta-hydroxysteroid	HSD11B1	P28845	CHEMBL	Enzyme	0.1115	141 / 8
N-(5-chloro)	Serine/threonine	CHEK1	O14757	CHEMBL	Kinase	0.1115	112 / 0
N-(5-chloro)	Serine/threonine	RAF1	P04049	CHEMBL	Kinase	0.1115	110 / 0
N-(5-chloro)	Serine/threonine	BRAF	P15056	CHEMBL	Kinase	0.1115	140 / 0
N-(5-chloro)	Lysine-specific	KDM4A	O75164	CHEMBL	Eraser	0.1115	1 / 0
N-(5-chloro)	Lysine-specific	KDM4C	Q9H3R0	CHEMBL	Eraser	0.1115	1 / 0
N-(5-chloro)	Metabotropic	GRM4	Q14833	CHEMBL	Family C	0.1115	3 / 16
N-(5-chloro)	G-protein-coupled	GPR84	Q9NQS5	CHEMBL	Family A	0.1115	6 / 0
N-(5-chloro)	Muscarinic	CHRM2	P08172	CHEMBL	Family A	0.1115	29 / 9
N-(5-chloro)	Arachidonic acid	ALOX15	P16050	CHEMBL	Enzyme	0.1115	19 / 0
N-(5-chloro)	Cyclin-dependent	CDK5R1	Q15078	CHEMBL	Kinase	0.1115	27 / 0
N-(5-chloro)	Dual-specific	DYRK1A	Q13627	CHEMBL	Kinase	0.1115	49 / 0
N-(5-chloro)	Phosphodiesterase	PDE10A	Q9Y233	CHEMBL	Phosphodiesterase	0.1115	45 / 0
N-(5-chloro)	Heat shock	HSP90AA	P08238	CHEMBL	Other cytochrome	0.1115	74 / 0
N-(5-chloro)	Glutamate	GRIN1	Q05586	CHEMBL	Ligand-gated	0.1115	18 / 0
N-(5-chloro)	Voltage-gated	CACNA2	P54289	CHEMBL	Calcium channel	0.1115	7 / 0
N-(5-chloro)	Beta amyloid	APP	P05067	CHEMBL	Membrane	0.1115	39 / 0
N-(5-chloro)	Histone deacetylase	HDAC1	Q13547	CHEMBL	Eraser	0.1115	255 / 91

Phytochemical	Target	Common Name	Uniprot ID	ChEMBL ID	Target Class	Probability	Known actives (3D)
N-(5-chloro-2-methyl-1,4-dioxane-6-yl)-N-methyl-2-pyrrolidone	Estradiol	HSD17B3	P37058	CHEMBL1205	Enzyme	0.1115	31 / 0
N-(5-chloro-2-methyl-1,4-dioxane-6-yl)-N-methyl-2-pyrrolidone	Transthyretin	TTR	P02766	CHEMBL1205	Secreted	0.1115	5 / 0
N-(5-chloro-2-methyl-1,4-dioxane-6-yl)-N-methyl-2-pyrrolidone	ALK tyrosine	ALK	Q9UM73	CHEMBL1205	Kinase	0.1115	12 / 0
Folic acid	Fatty acid	FABP4	P15090	CHEMBL1205	Fatty acid	1	5 / 4
Folic acid	Anandamide	FAAH	O00519	CHEMBL1205	Enzyme	1	6 / 17
Folic acid	Peroxisomal	PPARG	P37231	CHEMBL1205	Nuclear receptor	1	240 / 24
Folic acid	Peroxisomal	PPARA	Q07869	CHEMBL1205	Nuclear receptor	1	174 / 19
Folic acid	Telomerase	TERT	O14746	CHEMBL1205	Enzyme	1	1 / 2
Folic acid	Fatty acid	FABP5	Q01469	CHEMBL1205	Fatty acid	1	2 / 2
Folic acid	Peroxisomal	PPARD	Q03181	CHEMBL1205	Nuclear receptor	1	160 / 12
Folic acid	Fatty acid	FABP1	P07148	CHEMBL1205	Fatty acid	1	1 / 3
Folic acid	Acyl-CoA	SCD	O00767	CHEMBL1205	Enzyme	0.59204	11 / 1
Folic acid	Fatty acid	FABP3	P05413	CHEMBL1205	Fatty acid	0.56751	5 / 5
Folic acid	Protein-tyrosine	PTPN1	P18031	CHEMBL1205	Phosphatase	0.1661	119 / 60
Folic acid	T-cell protein	PTPN2	P17706	CHEMBL1205	Phosphatase	0.15793	39 / 20
Folic acid	Cyclooxygenase	PTGS1	P23219	CHEMBL1205	Oxidoreductase	0.14973	1 / 3
Folic acid	Free fatty acid	FFAR1	O14842	CHEMBL1205	Family A	0.14973	155 / 3
Folic acid	DNA topoisomerase	TOP1	P11387	CHEMBL1205	Isomerase	0.14152	1 / 3
Folic acid	HMG-CoA	HMGCR	P04035	CHEMBL1205	Oxidoreductase	0.14152	65 / 36
Folic acid	Prolyl endopeptidase	PREP	P48147	CHEMBL1205	Protease	0.13334	0 / 3
Folic acid	Protein-tyrosine	PTPN6	P29350	CHEMBL1205	Phosphatase	0.13334	1 / 1
Folic acid	Arachidonic acid	ALOX5	P09917	CHEMBL1205	Oxidoreductase	0.13334	22 / 23
Folic acid	Prostaglandin	PTGES	O14684	CHEMBL1205	Enzyme	0.13334	14 / 14
Folic acid	Phosphodiesterase	PDE4D	Q08499	CHEMBL1205	Phosphodiesterase	0.11697	33 / 1
Folic acid	Nuclear receptor	RORC	P51449	CHEMBL1205	Nuclear receptor	0.11697	0 / 10
Folic acid	Aldo-keto reductase	AKR1B1C	O60218	CHEMBL1205	Enzyme	0.11697	0 / 7
Folic acid	Dual specific	CDC25B	P30305	CHEMBL1205	Phosphatase	0.10877	4 / 6
Folic acid	Prostanoid	PTGER2	P43116	CHEMBL1205	Family A	0.10877	49 / 24
Folic acid	Leukotriene	LTB4R	Q15722	CHEMBL1205	Family A	0.10877	57 / 6
Folic acid	11-beta-hydroxysteroid	HSD11B1	P28845	CHEMBL1205	Enzyme	0.10877	27 / 42
Folic acid	Cytochrome	CYP19A1	P11511	CHEMBL1205	Cytochrome	0.10877	0 / 259
Folic acid	CD81 antigen	CD81	P60033	CHEMBL1205	Surface antigen	0.10058	0 / 1
Folic acid	Protein kinase	PRKCH	P24723	CHEMBL1205	Kinase	0.10058	0 / 1
Folic acid	LXR-alpha	NR1H3	Q13133	CHEMBL1205	Nuclear receptor	0.10058	6 / 20
Folic acid	Cyclooxygenase	PTGS2	P35354	CHEMBL1205	Oxidoreductase	0.10058	11 / 4
Folic acid	Dual specific	CDC25A	P30304	CHEMBL1205	Phosphatase	0.10058	16 / 16
Folic acid	Corticosteroid	SERPINA1	P08185	CHEMBL1205	Secreted	0.10058	0 / 23
Folic acid	Testis-specific	SHBG	P04278	CHEMBL1205	Secreted	0.10058	0 / 55
Folic acid	Glucose-6-phosphate	G6PD	P11413	CHEMBL1205	Enzyme	0.10058	0 / 7
Folic acid	Cytochrome	CYP51A1	Q16850	CHEMBL1205	Cytochrome	0.10058	0 / 2

Phytochemical	Target	Common	Uniprot ID	ChEMBL	Target Class	Probability	Known actives (3D)
Folic acid	Carboxylesterase	CES2	O00748	CHEMBL	Enzyme	0.10058	1 / 14
Folic acid	DNA polymerase	POLB	P06746	CHEMBL	Enzyme	0.10058	1 / 8
Folic acid	Receptor	PTPRF	P10586	CHEMBL	Membrane protein	0.10058	15 / 1
Folic acid	Protein-tyrosine phosphatase	PTPN11	Q06124	CHEMBL	Phosphatase	0.10058	16 / 2
Folic acid	Vanilloid receptor	TRPV1	Q8NER1	CHEMBL	Voltage-gated ion channel	0.10058	0 / 4
Folic acid	Glucocorticoid receptor	NR3C1	P04150	CHEMBL	Nuclear receptor	0.10058	28 / 36
Folic acid	Protein farnesyl transferase	FNTA	P49354	CHEMBL	Enzyme	0.10058	15 / 14
Folic acid	Niemann-Pick C1	NPC1L1	Q9UHC9	CHEMBL	Other membrane protein	0.10058	0 / 11
Folic acid	Sigma opioid receptor	SIGMAR1	Q99720	CHEMBL	Membrane protein	0.10058	0 / 4
Folic acid	Cytochrome P450	CYP17A1	P05093	CHEMBL	Cytochrome P450	0.10058	0 / 43
Folic acid	Low molecular weight GTP-binding protein	ACP1	P24666	CHEMBL	Phosphatase	0.10058	15 / 1
Folic acid	Prostanoid receptor	PTGIR	P43119	CHEMBL	Family A GPCR	0.10058	94 / 8
Folic acid	Androgen receptor	AR	P10275	CHEMBL	Nuclear receptor	0.10058	1 / 126
Folic acid	Phospholipase A2	PLA2G1E	P04054	CHEMBL	Enzyme	0.10058	1 / 1
Folic acid	Dopamine receptor	SLC6A3	Q01959	CHEMBL	Electrochemical transporter	0.10058	0 / 1
Folic acid	Adenosine deaminase	ADORA3	P0DMS8	CHEMBL	Family A GPCR	0.10058	0 / 3
Folic acid	MAP kinase	MAPK3	P27361	CHEMBL	Kinase	0.10058	0 / 1
Folic acid	Prostanoid receptor	PTGER1	P34995	CHEMBL	Family A GPCR	0.10058	20 / 12
Folic acid	Butyrylcholinesterase	BCHE	P06276	CHEMBL	Hydrolase	0.10058	0 / 2
Folic acid	Beta-secretase	BACE1	P56817	CHEMBL	Protease	0.10058	0 / 2
Folic acid	Nuclear receptor	NR1I3	Q14994	CHEMBL	Nuclear receptor	0.10058	0 / 2
Folic acid	DNA topoisomerase	TOP2A	P11388	CHEMBL	Isomerase	0.10058	0 / 2
Folic acid	Cannabinoid receptor	CNR1	P21554	CHEMBL	Family A GPCR	0.10058	3 / 24
Folic acid	11-beta-hydroxysteroid dehydrogenase	HSD11B2	P80365	CHEMBL	Enzyme	0.10058	2 / 19
Folic acid	Muscarinic acetylcholine receptor	CHRM2	P08172	CHEMBL	Family A GPCR	0.10058	0 / 1
Folic acid	Acetylcholinesterase	ACHE	P22303	CHEMBL	Hydrolase	0.10058	0 / 2
Folic acid	Norepinephrine transporter	SLC6A2	P23975	CHEMBL	Electrochemical transporter	0.10058	0 / 1
Folic acid	Serotonin transporter	SLC6A4	P31645	CHEMBL	Electrochemical transporter	0.10058	0 / 5
Folic acid	Cytochrome P450	CYP2C19	P33261	CHEMBL	Cytochrome P450	0.10058	0 / 4
Folic acid	Progesterone receptor	PGR	P06401	CHEMBL	Nuclear receptor	0.10058	4 / 46
Folic acid	Prostanoid receptor	PTGER4	P35408	CHEMBL	Family A GPCR	0.10058	56 / 9
Folic acid	Steroid 5-alpha-reductase	SRD5A2	P31213	CHEMBL	Oxidoreductase	0.10058	18 / 19
Folic acid	Bile acid receptor	NR1H4	Q96RI1	CHEMBL	Nuclear receptor	0.10058	126 / 9
Folic acid	Indoleamine 2,3-dioxygenase	IDO1	P14902	CHEMBL	Enzyme	0.10058	0 / 1
Folic acid	Nuclear receptor	RORA	P35398	CHEMBL	Nuclear receptor	0.10058	0 / 4
Folic acid	Nitric oxide synthase	NOS2	P35228	CHEMBL	Enzyme	0.10058	2 / 20
Folic acid	Fatty acid binding protein	FABP2	P12104	CHEMBL	Fatty acid binding protein	0.10058	1 / 1
Folic acid	Mineralocorticoid receptor	NR3C2	P08235	CHEMBL	Nuclear receptor	0.10058	2 / 23
Folic acid	Acyl coenzyme A oxidase	CES1	P23141	CHEMBL	Enzyme	0.10058	0 / 4
Folic acid	G-protein-coupled receptor	FFAR4	Q5NUL3	CHEMBL	Family A GPCR	0.10058	6 / 0

Phytochemical	Target	Common	Uniprot ID	ChEMBL	Target Class	Probability	Known actives (3D)
Folic acid	Phosphoc	PDE4A	P27815	CHEMBL	Phosphoc	0.10058	13 / 0Â Â Â Â Â
Folic acid	Phosphoc	PDE4B	Q07343	CHEMBL	Phosphoc	0.10058	37 / 0Â Â Â Â Â
Folic acid	Solute ca	SLC22A6	Q4U2R8	CHEMBL	Electroch	0.10058	0 / 2Â Â Â Â Â
Folic acid	Estrogen	ESR2	Q92731	CHEMBL	Nuclear re	0.10058	1 / 46Â Â Â Â Â
Folic acid	Squalene	FDFT1	P37268	CHEMBL	Enzyme	0.10058	3 / 6Â Â Â Â Â
Pentadec	Fatty acid	FABP4	P15090	CHEMBL	Fatty acid	0.67068	29 / 3Â Â Â Â Â
Pentadec	Peroxisor	PPARA	Q07869	CHEMBL	Nuclear re	0.67068	191 / 9Â Â Â Â Â
Pentadec	Fatty acid	FABP3	P05413	CHEMBL	Fatty acid	0.67068	14 / 5Â Â Â Â Â
Pentadec	Free fatty	FFAR1	O14842	CHEMBL	Family A	0.66158	159 / 3Â Â Â Â Â
Pentadec	Fatty acid	FABP5	Q01469	CHEMBL	Fatty acid	0.65259	4 / 2Â Â Â Â Â
Pentadec	Peroxisor	PPARD	Q03181	CHEMBL	Nuclear re	0.65259	142 / 7Â Â Â Â Â
Pentadec	Fatty acid	FABP2	P12104	CHEMBL	Fatty acid	0.65259	1 / 1Â Â Â Â Â
Pentadec	Solute ca	SLC22A6	Q4U2R8	CHEMBL	Electroch	0.1841	0 / 2Â Â Â Â Â
Pentadec	11-beta-h	HSD11B1	P28845	CHEMBL	Enzyme	0.1841	91 / 22Â Â Â Â Â
Pentadec	Dual spec	CDC25A	P30304	CHEMBL	Phosphat	0.14806	28 / 14Â Â Â Â Â
Pentadec	DNA poly	POLB	P06746	CHEMBL	Enzyme	0.13004	2 / 5Â Â Â Â Â
Pentadec	Prostano	PTGER2	P43116	CHEMBL	Family A	0.085	90 / 5Â Â Â Â Â
Pentadec	UDP-gluc	UGT2B7	P16662	CHEMBL	Enzyme	0.085	0 / 20Â Â Â Â Â
Pentadec	Cytochro	CYP19A1	P11511	CHEMBL	Cytochro	0.07597	0 / 22Â Â Â Â Â
Pentadec	Corticost	SERPINA	P08185	CHEMBL	Secreted	0.07597	0 / 6Â Â Â Â Â
Pentadec	Testis-sp	SHBG	P04278	CHEMBL	Secreted	0.07597	0 / 26Â Â Â Â Â
Pentadec	Estradiol	HSD17B3	P37058	CHEMBL	Enzyme	0.07597	0 / 11Â Â Â Â Â
Pentadec	Glucose-6	G6PD	P11413	CHEMBL	Enzyme	0.07597	0 / 9Â Â Â Â Â
Pentadec	GABA-B	GABBR1	Q9UBS5	CHEMBL	Family C	0.07597	0 / 1Â Â Â Â Â
Pentadec	G-protein	GPBAR1	Q8TDU6	CHEMBL	Family A	0.07597	5 / 15Â Â Â Â Â
Pentadec	Bile acid	NR1H4	Q96RI1	CHEMBL	Nuclear re	0.07597	96 / 11Â Â Â Â Â
Pentadec	Aldo-keto	AKR1B1C	O60218	CHEMBL	Enzyme	0.06698	2 / 7Â Â Â Â Â
Pentadec	Protein fa	FNTA FN	P49354	CHEMBL	Enzyme	0.06698	51 / 8Â Â Â Â Â
Pentadec	Vitamin D	VDR	P11473	CHEMBL	Nuclear re	0.06698	2 / 2Â Â Â Â Â
Pentadec	Lysine-sp	KDM2A	Q9Y2K7	CHEMBL	Eraser	0.06698	18 / 1Â Â Â Â Â
Pentadec	Lysine-sp	KDM5C	P41229	CHEMBL	Eraser	0.06698	19 / 1Â Â Â Â Â
Pentadec	Androgen	AR	P10275	CHEMBL	Nuclear re	0.06698	1 / 33Â Â Â Â Â
Pentadec	Niemann-	NPC1L1	Q9UHC9	CHEMBL	Other me	0.05796	0 / 6Â Â Â Â Â
Pentadec	GABA A	GABRA2	P47869	CHEMBL	Ligand-ga	0.05796	0 / 2Â Â Â Â Â
Pentadec	Histone ly	PHF8	Q9UPP1	CHEMBL	Eraser	0.04895	1 / 1Â Â Â Â Â
Pentadec	Prostano	PTGFR	P43088	CHEMBL	Family A	0.04895	1 / 1Â Â Â Â Â
Pentadec	Hydroxya	HAO1	Q9UJM8	CHEMBL	Enzyme	0.04895	4 / 1Â Â Â Â Â
Pentadec	11-beta-h	HSD11B2	P80365	CHEMBL	Enzyme	0.04895	16 / 3Â Â Â Â Â
Pentadec	Glutathior	GSTK1	Q9Y2Q3	CHEMBL	Enzyme	0.04895	0 / 1Â Â Â Â Â
Pentadec	Protein-ty	PTPN1	P18031	CHEMBL	Phosphat	0.04895	128 / 27Â Â Â Â Â

Phytochemical	Target	Common Name	Uniprot ID	ChEMBL ID	Target Class	Probability	Known actives (3D)
Pentadec	Retinoic acid	RARG	P13631	CHEMBL	Nuclear receptor	0.04895	122 / 0 0 0 0 0
Pentadec	Retinoic acid	RARB	P10826	CHEMBL	Nuclear receptor	0.04895	133 / 0 0 0 0 0
Pentadec	Retinoic acid	RARA	P10276	CHEMBL	Nuclear receptor	0.04895	122 / 0 0 0 0 0
Pentadec	Cytochrome	CYP26A1	O43174	CHEMBL	Cytochrome	0.04895	13 / 0 0 0 0 0
Pentadec	Retinoid	RXRRA	P19793	CHEMBL	Nuclear receptor	0.04895	167 / 0 0 0 0 0
Pentadec	Carbonic	CA1	P00915	CHEMBL	Lyase	0.04895	15 / 7 0 0 0 0
Pentadec	Carbonic	CA2	P00918	CHEMBL	Lyase	0.04895	9 / 5 0 0 0 0
Pentadec	Peroxisome	PPARG	P37231	CHEMBL	Nuclear receptor	0.04895	328 / 8 0 0 0 0
Pentadec	Retinoid	RXRB	P28702	CHEMBL	Nuclear receptor	0.04895	53 / 0 0 0 0 0
Pentadec	Retinoid	RXRG	P48443	CHEMBL	Nuclear receptor	0.04895	76 / 0 0 0 0 0
Pentadec	Transient	TRPA1	O75762	CHEMBL	Voltage-g	0.04895	1 / 0 0 0 0 0
Pentadec	G-protein	FFAR4	Q5NUL3	CHEMBL	Family A	0.04895	17 / 0 0 0 0 0
Pentadec	G protein	PTGDR2	Q9Y5Y4	CHEMBL	Family A	0.04895	524 / 0 0 0 0 0
Pentadec	Monocarbonyl	SLC16A1	P53985	CHEMBL	Electroch	0.04895	13 / 0 0 0 0 0
Pentadec	Plasma	RBP4	P02753	CHEMBL	Secreted	0.04895	13 / 0 0 0 0 0
Pentadec	Prostanoid	PTGER4	P35408	CHEMBL	Family A	0.04895	116 / 0 0 0 0 0
Pentadec	Voltage-g	CACNA2	P54289	CHEMBL	Calcium c	0.04895	0 / 4 0 0 0 0
Pentadec	HMG-CoA	HMGCR	P04035	CHEMBL	Oxidoreduct	0.04895	24 / 21 0 0 0 0
Pentadec	Nuclear	NR0B2	Q15466	CHEMBL	Nuclear	0.04895	1 / 0 0 0 0 0
Pentadec	Serotonin	HTR2B	P41595	CHEMBL	Family A	0.04895	2 / 0 0 0 0 0
Pentadec	Nuclear	RORB	Q92753	CHEMBL	Nuclear	0.04895	1 / 0 0 0 0 0
Pentadec	MAP kinase	MAPK1	P28482	CHEMBL	Kinase	0.04895	4 / 0 0 0 0 0
Pentadec	Nuclear	RORA	P35398	CHEMBL	Nuclear	0.04895	1 / 0 0 0 0 0
Pentadec	Oxoecic	OXER1	Q8TDS5	CHEMBL	Family A	0.04895	4 / 0 0 0 0 0
Pentadec	Arachidonic	ALOX15	P16050	CHEMBL	Enzyme	0.04895	3 / 0 0 0 0 0
Pentadec	Arachidonic	ALOX12	P18054	CHEMBL	Enzyme	0.04895	4 / 0 0 0 0 0
Pentadec	Prostaglandin	PTGES	O14684	CHEMBL	Enzyme	0.04895	59 / 8 0 0 0 0
Pentadec	Plasminogen	PLG	P00747	CHEMBL	Protease	0.04895	1 / 1 0 0 0 0
Pentadec	Cytochrome	CYP26B1	Q9NR63	CHEMBL	Cytochrome	0.04895	9 / 0 0 0 0 0
Pentadec	Cytosolic	PLA2G4A	P47712	CHEMBL	Enzyme	0.04895	60 / 0 0 0 0 0
Pentadec	Neuronal	CHRNA7	P36544	CHEMBL	Ligand-gate	0.04895	0 / 2 0 0 0 0
Pentadec	Thromboxan	TBXA2R	P21731	CHEMBL	Family A	0.04895	196 / 0 0 0 0 0
Pentadec	Aldo-keto	AKR1C1	Q04828	CHEMBL	Enzyme	0.04895	1 / 0 0 0 0 0
Pentadec	Prostanoid	PTGDR	Q13258	CHEMBL	Family A	0.04895	157 / 0 0 0 0 0
Pentadec	Metabotropic	GRM5	P41594	CHEMBL	Family C	0.04895	0 / 4 0 0 0 0
Pentadec	Epoxide	EPHX2	P34913	CHEMBL	Protease	0.04895	61 / 0 0 0 0 0

5.7.5 VENNY 2.1 DATABASE OF KAPPAPHYCUS AND GRACILARIA :

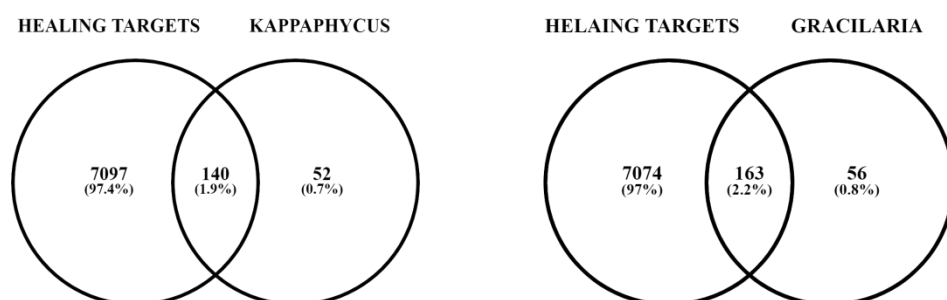


Fig 5.7.5 Venn diagram of healing targets with kappaphycus and gracilaria

From figure 5.7.5 the wound healing targets and kappaphycus, gracilaria has common targets Kappaphycus has 140 targets and gracilaria has 163 targets which is shown in Venn diagram.

5.7.6 COMMON TARGETS FOR KAPPAPHYCUS AND GRACILARIA :

The common of kappaphycus and gracilaria has taken from veny2.1 software where play important role in network pharmacology.

S.NO	KAPPAP	GRACILARIA	S.NO	KAPPAP	GRACILARIA	S.NO	KAPPAP	GRACILARIA
1	MMP1	MMP1	41	PRKCB	ACP1	81	DRD5	IDO1
2	MMP9	CXCL8	42	CDK5	EDNRA	82	TOP2A	GABBR1
3	MMP2	MMP9	43	KIT	CYP19A1	83	KCNH2	MAOA
4	EGFR	MMP2	44	NR1I2	CMA1	84	PDE4A	CSNK2A1
5	PLEC	PLG	45	NR1H2	ECE1	85	PRKCQ	RARB
6	AKT1	MMP13	46	G6PD	PRKCD	86	FABP5	TOP2A
7	FGFR1	MMP8	47	VDR	ESR1	87	PIM1	MCL1
8	PTK2	MAPK1	48	HSD11B1	MME	88	ALDH2	CTSA
9	NR3C1	MMP3	49	RET	HNF4A	89	SLC6A3	PDE4A
10	FGFR3	CTNNB1	50	TRPV1	CNR2	90	CYP2C19	HSP90AB1
11	F3	NR3C1	51	CYP51A1	AGTR2	91	CA4	TRPM8
12	KDR	MAPK14	52	CCR1	G6PD	92	PRKCH	FABP5
13	MET	TTR	53	TACR2	VDR	93	SPHK1	AKR1A1
14	NOS2	SRC	54	PTPN6	HDAC6	94	RPS6KA1	HDAC2
15	ALOX5	NOS2	55	SERPINA1	PLA2G4A	95	PRKCG	KDM4A
16	NTRK1	BCL2	56	ESR2	HSD11B1	96	PRKD1	SLC6A3
17	PRKCE	ALOX5	57	BCHE	RET	87	AKR1B1	CCKBR
18	ERBB2	MPEG1	58	CYP3A4	TRPV1	98	ALOX12	CYP2C19
19	PPARG	MAPK8	59	PTGS1	CYP51A1	99	DRD2	PRKCH
20	PTGS2	PPARG	60	GLI1	APP	100	FABP1	AKR1B1
21	GSK3B	PTGS2	61	PTGER4	VCP	101	FABP2	ALOX12
22	MAPK3	MAPK3	62	NR3C2	PTPN6	102	AR	GPBAR1
23	PPARD	ITGAV	63	SLC6A4	ENPP2	103	GLI2	FABP1
24	ACHE	BRAF	64	TERT	SERPINA1	104	ALK	FABP2
25	FLT1	PPARD	65	ADORA3	ESR2	105	LRRK2	AR
26	NOX4	ACHE	66	CTSK	BCHE	106	FAAH	BCL2L1
27	PPARA	ADAMTS	67	NOX1	CYP3A4	107	AKR1B10	ALK
28	CFTR	PPARA	68	HSD11B2	PTGS1	108	FABP3	FAAH
29	IGF1R	CHRNA7	69	HDAC1	P2RX7	109	SRD5A1	RBP4
30	PTPN1	CTSG	70	PTGER2	PTGER4	110	LTB4R	AKR1B10
31	ALOX15	RAF1	71	DBH	NR3C2	111	TYR	FABP3
32	PTPN11	CCR2	72	HMGCR	SLC6A4	112	PDPK1	SRD5A1
33	AURKA	MDM2	78	CYP17A1	TERT	113	TOP1	LTB4R
34	CD81	ACE	74	CYP11B1	ADORA3	114	ADRA1D	LDHA
35	SRD5A2	PTPN1	75	CNR1	HSD11B2	115	SREBF2	PDPK1
36	ACP1	AGTR1	76	IDO1	HDAC1	116	PDK1	TOP1
37	CYP19A1	ALOX15	77	ACVR1	PTGER2	117	SQLE	SLC16A1
38	PRKCD	PTPN11	78	GSK3A	HMGCR	118	PTGER1	KDM5B
39	ESR1	CD81	79	CSF1R	CYP17A1	119	AURKB	PFKFB3
40	SHH	SRD5A2	80	PRKCZ	ACP2	120	SCD	SREBF2

S.NO	KAPPAP	GRACILAS	S.NO	GRACILA
121	TRPA1	OXER1	144	RORA
123	NR1H3	DYRK1A	145	THRB
124	PTPN2	HDAC3	146	WEE1
125	PYGL	AKR1C3	147	CACNA2I
126	FABP4	PTGER1	148	CDC25A
127	CA2	CHEK1	150	CHRM2
128	PDE4D	SCD	151	FTO
130	PGR	RXRA	152	RARG
131	RORA	TRPA1	153	THRA
132	CDC25A	NR1H3	154	KDM5C
133	CHRM2	PTPN2	156	LDHB
134	FTO	PTGFR	157	MAP3K8
135	PLK4	FABP4	158	PDE4B
138	CA9	KDM2B	159	AKR1C1
139	PTK6	HAO1	160	AMPD3
140	PDE4B	KDM4C	161	CYP26A1
141	SPHK2	CA2	162	HTR2B
142	HTR2B	RARA	163	KDM5A
143	CA6	TBXA2R	164	HSD17B1
144	HSD17B1	IMPDH2	165	KDM2A
143	FFAR4	PDE4D	166	FFAR4

5.7.7 NETWORK PHRAMACOLOGY OF KAPPAPHYCUS AND GRACILARIA :

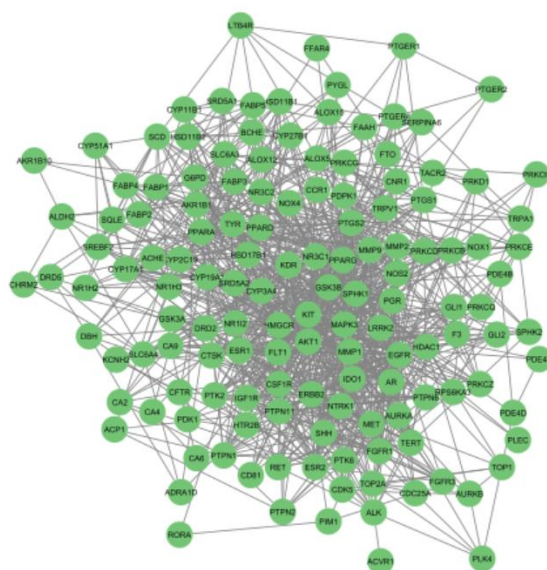


Fig 5.7.7.1 Network of kappaphycus targets

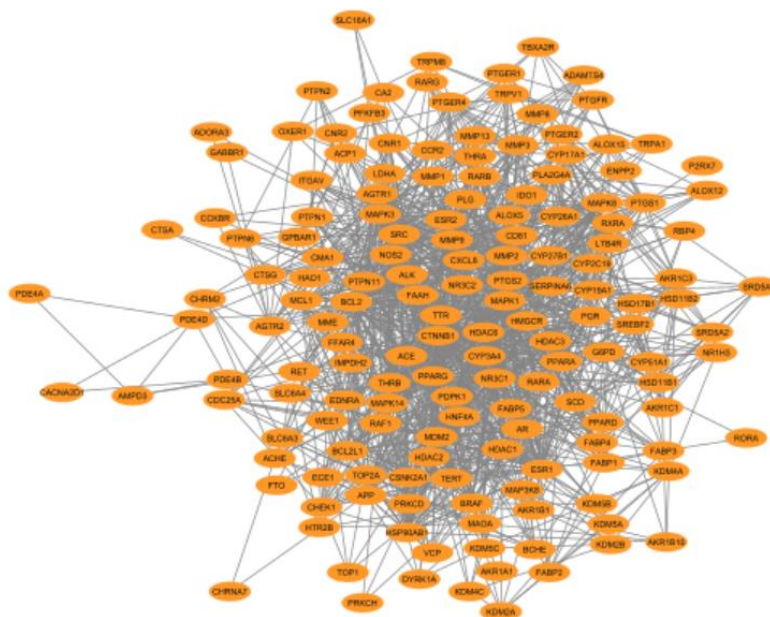


Fig 5.7.8.2 Network of gracilaria targets

5.7.8 TOP 10 TARGETS FOR MOLECULAR DOCKING IN KAPPAPHYUCUS AND GRACILARIA :

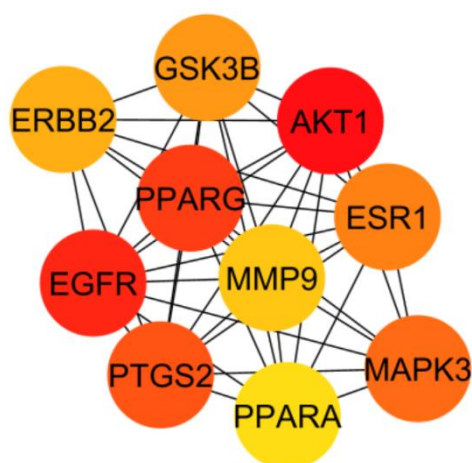


Fig 5.7.9.1 Top 10 Targets in K_p

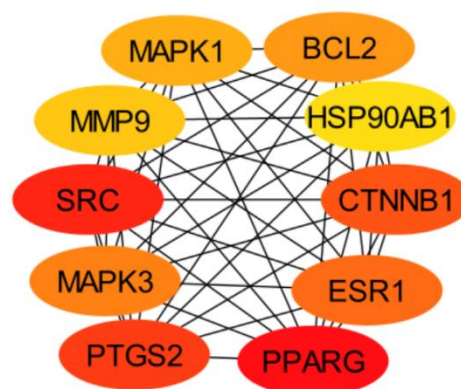


Fig 5.7.9.2 Top 10 Targets in G_R

5.8 MOLECULAR DOCKING :

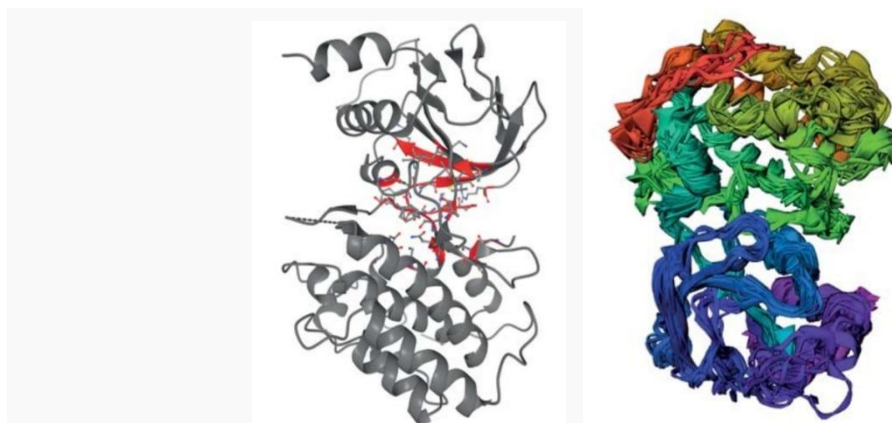


Fig 5.8.1 DOCKING IMAGE OF KAPPAPHYCUS

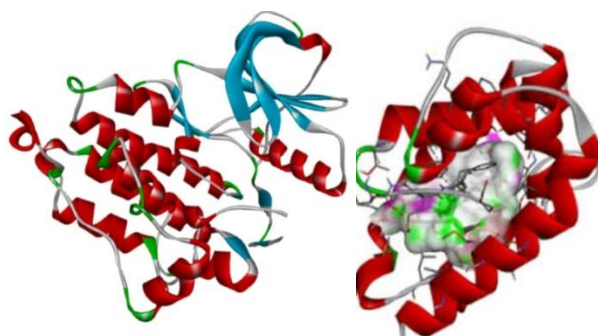


Fig 5.8.2 DOCKING IMAGE OF GRACILARIA

CHAPTER – 6

SUMMARY AND CONCLUSION

Hydrogels have emerged as attractive materials for wound healing applications because to their distinct features, which include high water content, biocompatibility, and variable mechanical properties. In recent years, there has been an increased focus in designing hydrogel formulations that can promote accelerated wound healing by including bioactive chemicals and gaining a better knowledge of the molecular principles that underpin the healing process. Bioactive compound kappaphycus and gracilaria such as growth factors, antimicrobial agents, and anti-inflammatory agents, help to promote wound healing by influencing numerous cellular processes involved in tissue repair. These chemicals can be used with hydrogel formulations to enable continuous release at the wound site, increasing their therapeutic effectiveness. For example, growth factors such as platelet-derived growth factor (PDGF) and vascular endothelial growth factor (VEGF) have been demonstrated to enhance cell proliferation and angiogenesis, resulting in faster wound closure. In conclusion, incorporating bioactive chemicals and mechanistic insights into hydrogel formulations is a viable strategy for enhancing wound healing therapy. Hydrogels can be adjusted to give increased effectiveness and encourage quicker healing by meticulously designing them and studying the underlying biological mechanisms involved in wound repair. These hydrogels, which include bioactive substances such as growth factors, antimicrobial agents, and anti-inflammatory agents, can address several aspects of the wound healing cascade, including cell proliferation, angiogenesis, and tissue regeneration. Furthermore, the discovery of mechanistic insights into the interactions between hydrogel components and the wound milieu enables the creation of more tailored and effective formulations. Moving forward, more study in this sector will continue to increase our understanding of wound healing mechanisms and enable the creation of novel hydrogel-based therapeutics with superior clinical results. Finally, the combination of bioactive chemicals with mechanistic insights shows enormous promise for the future of wound care, providing patients with shorter healing periods, a lower chance of infection, and a higher overall quality of life.

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ANNEXURE

GATE ADMIT CARD :

		GRADUATE APTITUDE TEST IN ENGINEERING 2024 अभियांत्रिकी स्नातक अभिक्षमता परीक्षा २०२४ ORGANISING INSTITUTE: INDIAN INSTITUTE OF SCIENCE, BENGALURU	
ADMIT CARD			
Name of the Candidate		SADHANA V	
Registration Number	BT24S57402260		
Paper Code/Name	BT : Biotechnology		
Date	10th February 2024 (Saturday)		
Time	9:30 AM to 12:30 PM		
Session	Forenoon : S5		
Photo ID Submitted	PAN Card (Number : CPNPV5890R)		
Examination Centre Code: 7402			
Address of the Centre:		V. Sadhana	
ION Digital Zone IDZ Kovilambakkam Center 2, Fortune Towers, 1st and 2nd Floor, SH 109, 200 Feet Thoraiappakkam Pallavaram Radial Road, Near Eachangadu signal, Chennai, Tamilnadu, PIN : 600117, India.			
			
Prof. Chandra Sekhar Seelamantula Organising Chairperson, GATE 2024 (on behalf of NCB-GATE, for MoE)		T500X40 66E3FAA2D1EF898AE2053185033585B53	
INSTRUCTIONS TO CANDIDATES			
1. An electronic copy of the Admit Card is NOT acceptable. A printed copy of the Admit Card must be presented for verification along with the original valid photo identification document submitted at the time of application. In case the quality of the photograph on the identification document is poor, the candidate must bring an additional recent valid photo ID (Aadhaar Card, Driving License, PAN Card, Passport and Voter ID). 2. To facilitate the identity verification by the Examination Centre personnel, candidates are advised to report to the examination venue at least 90 minutes before the scheduled commencement of the examination. Candidates will NOT BE ALLOWED to login 30 minutes after the start of the exam. 3. Candidates will be permitted to occupy their seats before the scheduled start of the examination. Candidates can login and start reading the instructions 20 minutes before the start of the examination. 4. During the examination, a virtual scientific calculator will be available on the candidate's computer. 5. Personal calculators, mobile phones, watches of any kind or any other electronic devices are prohibited inside the Examination Centre. Charts, tables, papers, books, sheets and heavy ornaments are also not allowed inside the Test Centre. 6. A scribble pad will be provided for rough work. Candidates must write their name and Registration number on the scribble pad before using it. A candidate can possess only one scribble pad at any point of time. If the scribble pad gets filled, candidates can ask for another scribble pad, after returning the previous one to the invigilator. A scribble pad once surrendered will not be returned to the candidate. At the end of the examination, the scribble pad in possession of the candidate must be returned to the invigilator. 7. Candidates must bring their own pen and pencil. Candidates are also allowed to bring a transparent water bottle. 8. Candidates are not allowed to bring any items other than those mentioned above. Examination Centre personnel are not responsible for the safety of the candidate's personal belongings. Candidates in possession of prohibited items will be deregistered, debarred from the examination, and may also be banned from appearing in future GATE examinations. 9. Candidates will not be allowed to leave the examination hall before the end of the examination. 10. Impersonation and violation of the above guidelines or the Code of Conduct as given in the Information Brochure will lead to cancellation of candidature and attract penal action. 11. PwD candidates are advised to bring their assistive devices, if any, and show them to the Examination Centre personnel for scrutiny. 12. PwD candidates who have been granted one-hour compensatory time in GATE 2024 examination are allowed to leave the examination hall after 12:30 PM in the forenoon session and after 5:30 PM in the afternoon session, by clicking the SUBMIT button only in the presence of the Invigilator. Once they click the SUBMIT button, the responses will be frozen, and the exam will end for them.			



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