

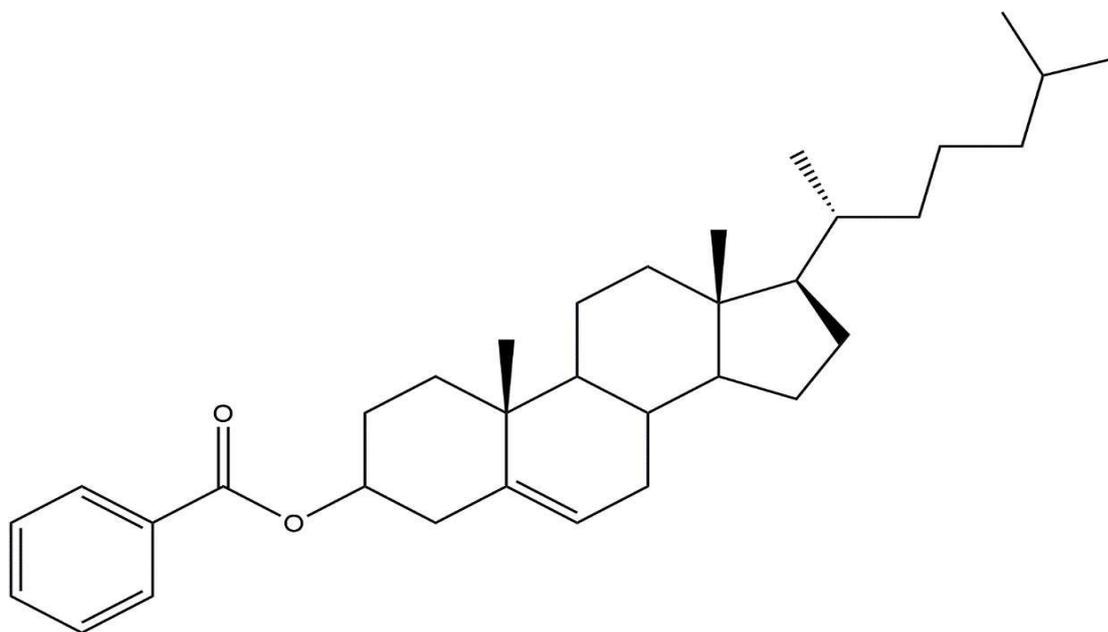
# **Chapter I**

## **Introduction**

## 1.1. Antiquity and Development of Liquid Crystals

The types and ordering of elements within each of the common forms of substance are the primary differences between them. Positional order and orientation order are present in the molecule that forms a crystalline solid with high order. On the other hand, certain substances exhibit intermediate states that are less ordered than conventional crystals but more ordered than liquids. Liquid crystals are these organized fluids. In this form, a liquid crystal material has the flowing characteristics of a liquid but exhibits strong anisotropy in some of its characteristics, such as the birefringence linked to crystalline solids [1].

Friedrich Reinitzer, an Austrian botanist, observed in 1888 that cholesterol benzoate had a peculiar melting behavior that showed two melting points when heated (Figure 1.1). The rigid ester melted first at 145.5 °C, forming a cloudy material that disappeared and transformed into a transparent isotropic liquid at 178.5 °C. [2]. Using a polarizing microscope, Lehmann examined the material of Reinitzer and established the presence of “liquid crystal” [3].



**Figure 1.1:** Structure of Cholesteryl benzoate

Vorlander conducted a thorough investigation of the relationship between mesogen characteristics and chemical species in 1908 [4]. Numerous research teams have examined numerous homologous series and methodically altered the shape of the aromatic nucleus, which alters the temperatures of the compounds [5-8]. Research by S. Chandrasekhar and associates from 1977 [9] described how disc-like molecules can form liquid crystals. The discotic nematic phase was observed in the hexa-substituted benzene derivatives that they synthesized. A brief

description of the developments in this field, with special attention to the structural elements, was noted [10]. The development of discotic liquid crystals on triphenylene was investigated by S.K. Pal *et al.* [11]. A review by Tobias Wohrle *et al.* on discotic liquid crystals is compelling [12]. The unique ferroelectric behavior of liquid crystals in a banana form is reported by Niori *et al.* [13]. Ros *et al.* examine the key ideas of bow-shaped compounds. A review on bent-core liquid crystals, including banana-shaped ones, was reported by Michael Hird [14, 15]. In contrast, LC phases have a regular repeating order. An elongated polymer solution could potentially behave as mesogenic materials, according to Flory's 1956 prediction [16]. A review of liquid crystalline polyazomethine polymers was described by Hussein *et al.* [17]. A detailed overview of liquid crystalline polymers was recently published by Lyu X *et al.* [18].

## 1.2. Birefringence in Liquid Crystals

The refractive index, or  $n$ , determines how quickly light moves through transparent materials with an isotropic structure. High-refractive index materials allow light to pass through more slowly, while lower index materials allow light to pass through more quickly. On the other hand, an anisotropic molecular structure of a material will result in an anisotropic refractive index. As a result, light moves through these materials at a variable speed in different directions. These materials are referred to as birefringent. Birefringence, commonly referred to as Double Refraction, is a characteristic of liquid crystals as well as a naturally occurring material found in solids like calcite. To be more accurate, materials that exhibit birefringence will exhibit varying refractive indices with respect to both direction and polarization.

## 1.3. Classification of Liquid Crystals

Figure 1.3 shows the general classification of liquid crystals. Based on their chemical structure, thermotropic and lyotropic liquid crystals are the two main categories into which liquid crystals are most commonly classified.

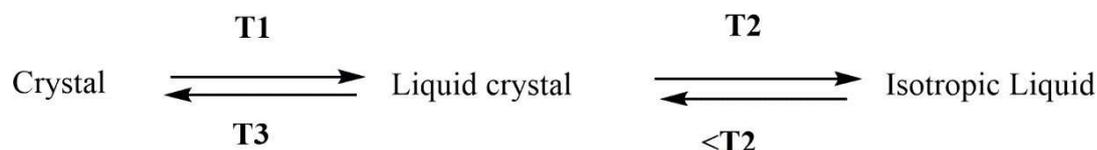
### 1.3.1 Thermotropic liquid crystals:

The term "thermotropic liquid crystal" refers to a chemical whose behavior mostly depends on temperature and exhibits a liquid crystalline condition [19]. Within a specific temperature range, thermotropic fluid crystals form. The material will become an isotropic fluid if the temperature increases too much and hence thermal motion will disrupt the molecular order.

Different forms of thermotropic liquid crystals:

### 1.3.1.1 Enantiotropic Liquid Crystals:

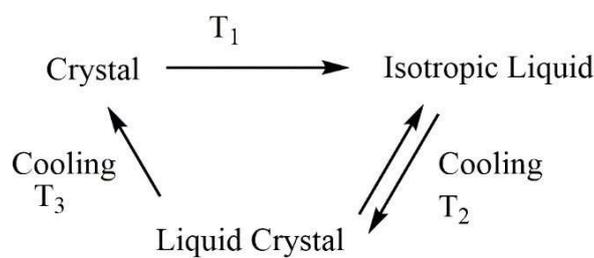
By reversibly heating and cooling the solid, this phenomenon is known as enantiotropic, and the material is known as enantiotropic.



where  $T_2 > T_1 > T_3$

### 1.3.1.2 Monotropic Liquid Crystals:

When a compound is heated and cooled at a certain temperature and it shows mesomorphic behaviour in any one of the cycles, then it is termed a monotropic liquid crystals.

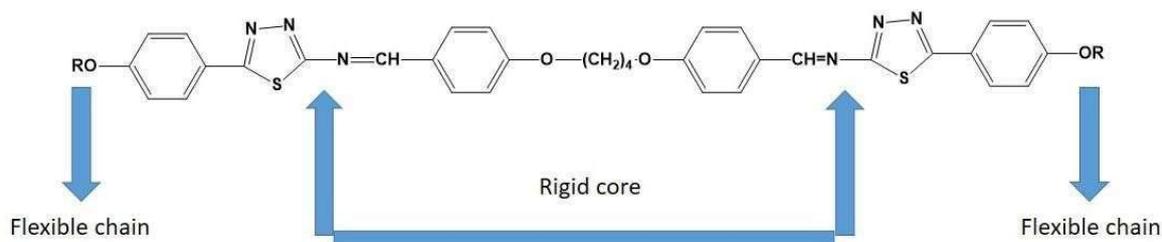


where  $T_1 > T_2 > T_3$

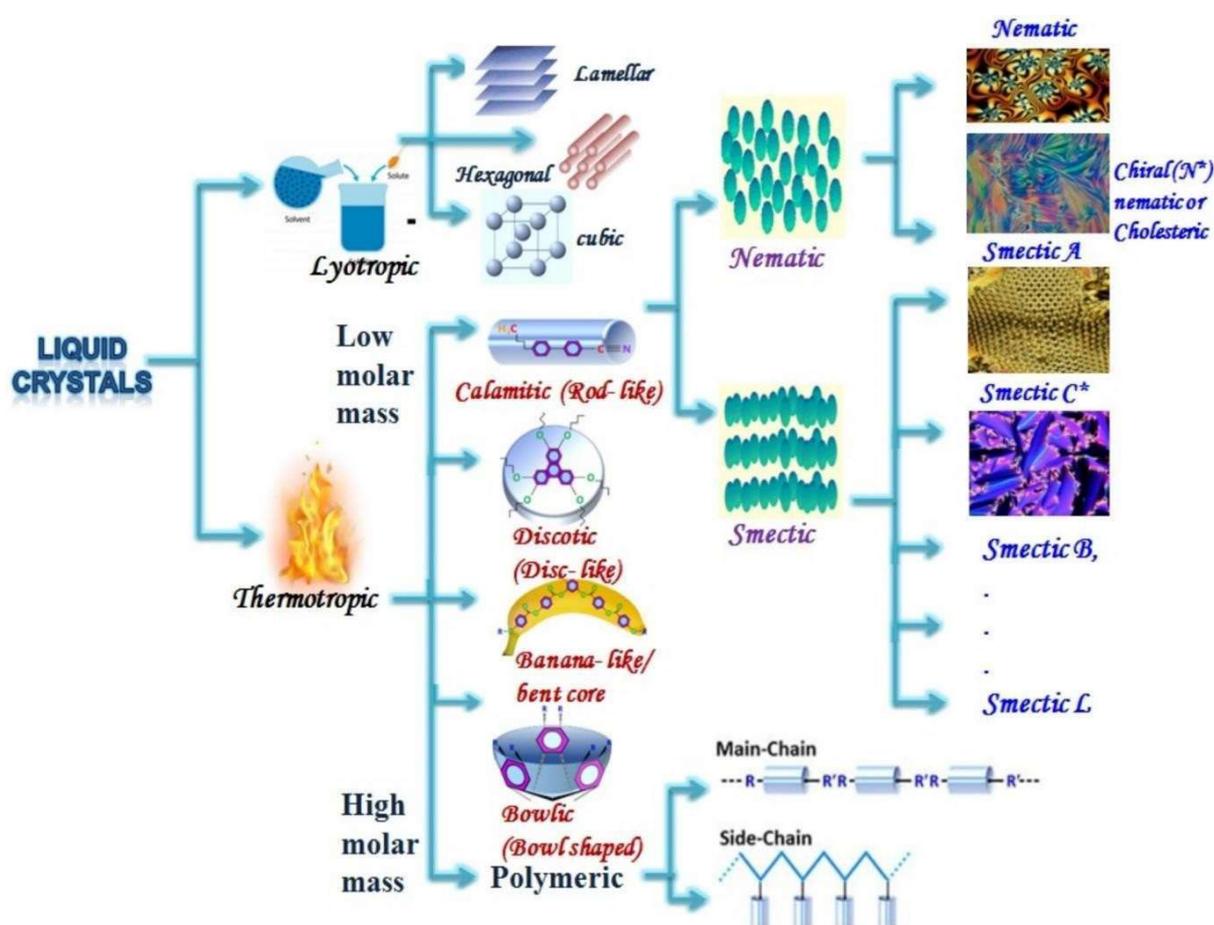
The three kinds of thermotropic liquid crystals are based on the molecular shape of the mesogens.

### 1.3.1.3 Rod-like structure:

The most prevalent type of compound that forms the elongated shape, which has significant differences that provide the necessary anisotropy. These substances are "calamitic liquid crystals". Since the calamitic mesogen needs to stay elongated to induce directed interaction, it typically has a stiff central core. Rigid connecting groups exist in linear chains. The majority of elongated compounds consist of more rings joined together either with the help of a connecting group.



**Figure 1.2:** Representative diagram of calamitic liquid crystal



Courtesy: <https://images.app.goo.gl/stuGrvm8VhoAJE6FA>

**Figure 1.3:** Representative Categorization of Liquid Crystals

Calamitic mesogenic materials fall into two groups according to the molecular configuration in different mesophases:

### a. Smectic Phase:

Since the mesophase is a thick, turbid liquid with soapy qualities, Friedel named the term smectic [20]. The most ordered phase of liquid crystals is called smectic mesophase. The long molecules in the smectic mesophase are stacked, parallel to one another, and grouped in a layered form. It tends to produce a sequence of terraces or layers when applied on a horizontal surface. The plain of Granjana is the name given to these terraces [21]. The molecular cohesion of the smectic liquid crystal is broken by heating, but not enough to cause the lateral binding to disintegrate, so the layers essentially stay intact. The smectic phase appears as rod-shaped, birefringent droplet particles after cooling. These rods have a focused cone texture that is typical of the smectic mesophase, and their number increases with decreasing temperature [22, 23]. Nevertheless, SmA and SmC are the most researched smectic phases. Each layer's molecules are organized vertically in the smectic-A, with an uneven arrangement in the core that results in a liquid state. These layers have a fair amount of glide. This phase possesses fluid qualities as a result. A skewed or tilted version of smectic-A is called smectic-C. About the layer, the molecules are angled.



**Figure 1.4:** Focal conical texture of Smectic A phase

### Twist Grain Boundary (TGB) Phase:

In certain chiral materials, a disordered mesogenic phase known as the Twist-Grain Boundary Phase (TGBA\*) has been predicted and found [24-27]; it occurs at a temperature higher than the typical layered phases. The non-helical SmA phase serves as the foundation for this frustrated phase structure. At the same time, the creation of a helix is enhanced by the significant asymmetry that manifests in the TGBA\* phase. The SmA phase is divided into modular in the TGBA\* phase structure by screw dislocations that cause the molecular director of the subsequent block to twist sharply at a smaller angle. This twining proceeds throughout

to form a spiral structure. Consequently, SmA leads initially to the microscopic phase structure; but, as the screw dislocation progresses, SmC takes over, and a nematic phase structure is formed. The TGBA\* features a double helix structure since the screw dislocation is helical as well.

### **Smectic C\* Phase:**

An asymmetric equivalent of the SmA phase is called chiral smectic C phase. The structure of the molecules remains unchanged, and the direction changes gradually and slightly (the tilt angle concerning the normal layer remains unchanged). In the case of chiral tilted molecules in the SmC phase, a primitive cell's symmetry is decreased to a dihedral axis. Despite the molecule's rapid reorientation motion, the overall result of this severe reduction in symmetry is a disparity in the dipole moment along the C2 axis. An impulsive polarisation is produced by this dipole in equivalence, and its direction varies as the helix's tilt direction changes. Because Ps is essentially nil, the phase can be accurately described as helielectric. Unwinding the spiral produces a real polar phase, though, since only one layer of the chiral smectic C phase is ferroelectric [24].

### **Ferro, antiferro, and ferrielectric chiral Smectic C phases:**

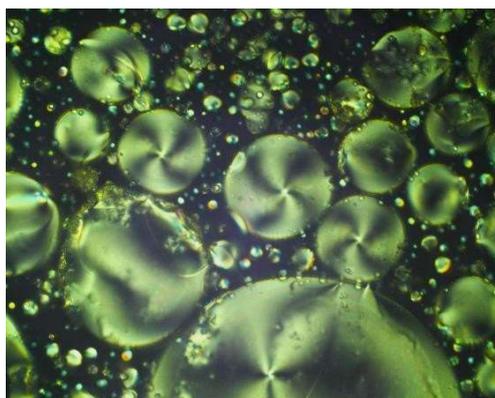
Ferroelectric characteristics are present in all the tilting smectic phases. Ferroelectric liquid crystals are so named because of their poor symmetry, which allows them to display spontaneous polarisation and piezoelectric characteristics. An inclined substance is known to have a permanent electric polarisation P that is similar to the smectic plane and upright to the director. The interactions between molecules and with any applied electric field or cell wall are substantially changed when permanent dipoles are present. When shifting from one layer to the next, there is an angle rotation in the slant direction. Either a left- or right-handed helix forms as a result of the continuous rotation. The type of chiral center and its orientation with the other mesogenic material's central core define the helical twist sense. Two other related phenomena are the antiferroelectric and ferrielectric phases [25–27]. The molecular layers in an antiferroelectric SmC\* phase are stacked so that the polarisation directions in each succeeding stratum point in the reverse directions, resulting in spontaneous polarisation of zero.

Layers are arranged in such a way that there is an impulsive polarisation in a ferrielectric smectic phase. There is an unequal number of opposite polarisation layers. For instance, there can be doubled the structure if the polarization order of one sort of layer is different from that of the other. Additionally, it has been proposed that there are two interpenetrating sublattices

in the layer stacking. For most of the phase, there will be alternating layer structures, meaning that two levels will be slanted to the right and one to the left. As a result, there will be detectable polarisation in the ferroelectric phase.

### **b. Nematic Phase:**

It exhibits a thread-like structure, the term "nematic" is derived from the Greek word "nema," which is termed as thread. The molecules are not stratified instead, they are aligned to the principal axis. Molecules are grouped, with roughly 100,000 molecules in each group. These clusters were referred to as "Swarms." E. Bose [24] initially put forth the group theory in 1909 in an attempt to describe mesomorphic behavior. The nematic phase's characteristics show that the molecules are always moving, which means that rather than the swarms staying stationary, the molecules will be exchanging information with one another. The swarms non-rigid configuration will be impacted by mechanical deformation. Because it is so fluid, the nematic phase has a low viscosity. From the perspective of characteristics like susceptibility, they are anisotropic [25]. In the melt, nematic crystals split into spherical droplets, which combine to form the threaded structure. The director is the preferred direction that the long molecular axis typically points in [26]. Figure 1.5 illustrates the nematic compound has a threaded texture when viewed under POM. Nematic fluid is identical to isotropic fluid in terms of fluidity, but it is more easily aligned with external magnetic or electric forces. Because they possess the optical characteristics of uniaxial crystals, aligned nematics are highly advantageous.

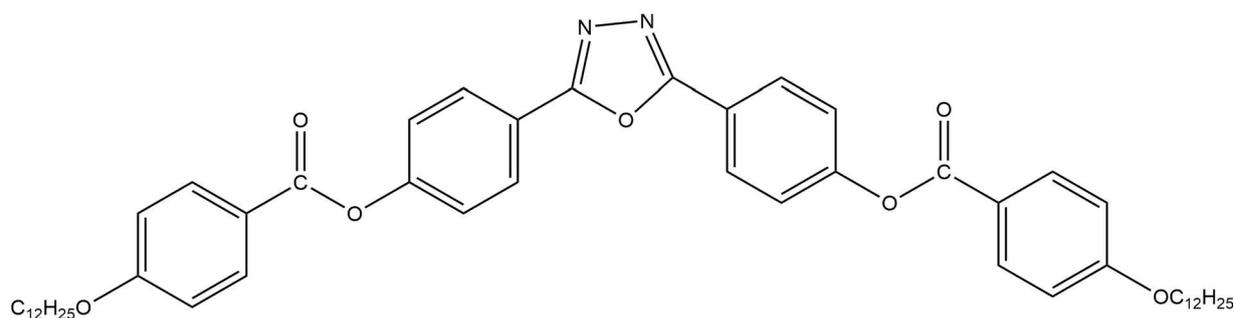


**Figure 1.5:** Typical marbled-like texture of the Nematic phase

### **Biaxial Nematic Phase:**

A structured homogenous mesogen with three separate principal axes is called biaxial nematic. This is in contrast to a simple nematic, where the system is rotationally symmetric around a single chosen axis. A biaxial nematic has the symmetry group  $D_{2h}$ , which is equivalent to a

right prism with three vertical mirror planes and three vertical  $C_2$  axes. In 2004, the first report of a thermotropic biaxial nematic was published [28, 29]. It was based on an oxadiazole bent-core mesogen with a boomerang-like form. This compound's biaxial nematic phase only appears at temperatures of about 200 °C, and it is preceded by unidentified smectic phases. Additionally, it has been discovered that this substance can divide into opposite-handed asymmetric domains [30]. The molecules with the boomerang shape take on a helical superstructure for this to occur.



**Figure 1.6:** Oxadiazole bent core mesogen

As predicted by theory and simulation [31], a temperature change from one-dimensional to two-dimensional mesophase is seen in one azo bent-core mesogen [29]. After heating from the  $N_u$  phase, this transition is seen in X-ray diffraction when the nematic reflection splits, and in Polarising optical microscopy as a shift in Schlieren texture and increased light transmittance. Since the transition involves low energy content and second-order, differential scanning calorimetry (DSC) is unable to detect it. The translational order variables for the uniaxial nematic phase are 0.75 to 1.5 times the mesogen length and for the biaxial nematic phase 2 to 3.3 times the mesogen length [32-34]. Combining disc-like discotic mesogens and classical rod-like mesogens is another method for achieving biaxial nematics. It is believed that the biaxial nematic phase will be situated beneath the rod-disc phase diagram minimum. Although the biaxial nematic phase is still elusive, a homogenous system of discs is observed in one study [19].

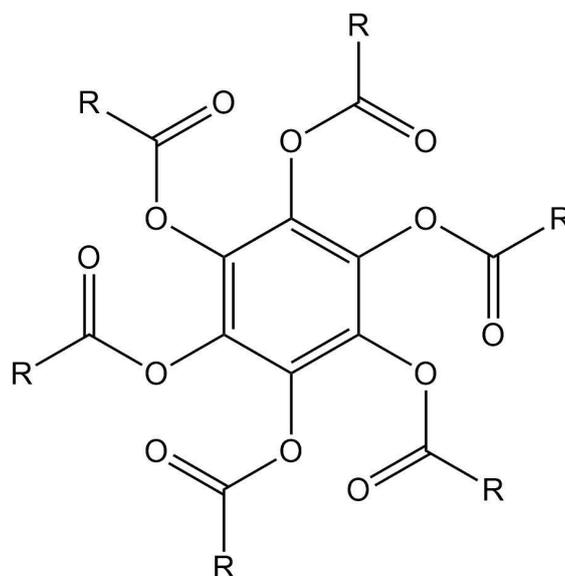
### Chiral Nematic ( $N^*$ ) Phase:

The chiral center of nematic mesogenic molecules, which develops weak chemical forces that enhances molecular arrangement which usually makes up the chiral nematic (also known as cholesteric) liquid crystal phase. Pitch is a significant feature of the chiral nematic mesophase. The ability of the chiral nematic phase to selectively reflect light with a frequency equal to

pitch length is a result of its helical structure. When the pitch equals the appropriate wavelength of light in the visible spectrum, a colour is reflected. The effect is based on the thermal dependency of the pitch length modification caused by the progressive arrangement between layers which changes the wavelength of reflected light in response to temperature. By increasing the molecule temperature and providing it with additional thermal energy, it is possible to tighten the pitch and increase the angle at which the director changes. Similarly, the distance between adjacent mesogenic materials increases as the molecule's temperature drops. This enables the formation of a liquid crystal thermometer whose reflected colour indicates the temperature of its surroundings. It is very common to combine different kinds of these liquid crystals to build sensors that react differently to temperature changes. These sensors are used in thermometers, frequently as thermosensitive films which are used to identify problems with battery health, radiation levels, and new products like "mood" rings.

#### 1.3.1.4 Disc-like structure:

Discotic liquid crystals are disc-like mesogens. The disc-shaped mesophase [35] was initially identified in 1977 by Indian scientists S. Chandrasekhar *et al.* (Figure 1.7). Three to eight flexible chains surround a central aromatic functionalized core in a typical discoid mesogen. Nematic and columnar phases are the two main forms of discotic liquid crystals. Although the disc's axis is more or less pointing in the same direction in this instance, the discotic nematics structure is comparable to that of the calamitic nematics.

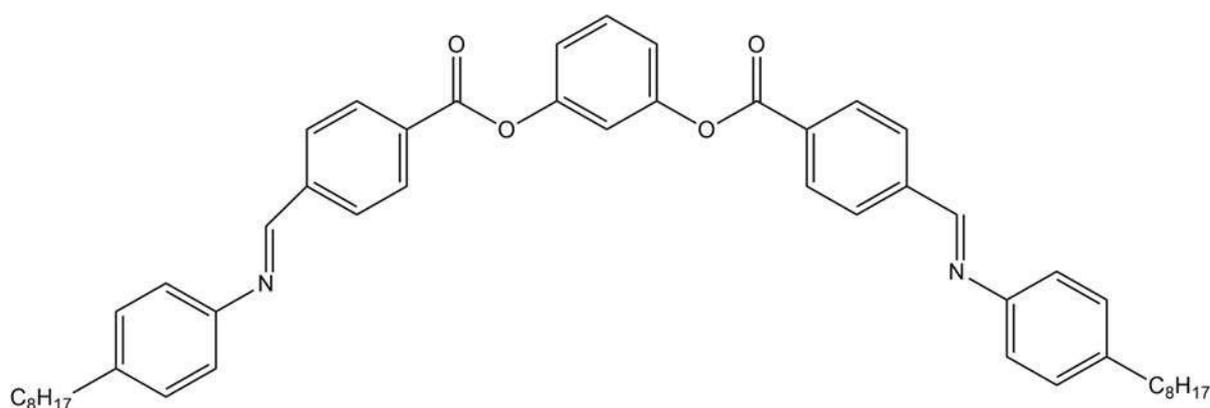


Where R =  $-C_4H_9$  to  $-C_9H_{19}$

**Figure 1.7:** Example of discotic liquid crystal

### 1.3.1.5 Banana-like structure:

Banana-shaped mesogens is the name for bow-shaped materials. Initially, the bent-core LC is synthesized by Vorlander [36]. Ferroelectric characteristics were reported by Niori *et al.* [13]. Because of their morphology and polarization effect, banana-shaped mesogens develop a complex, layered structure and are the only material in liquid crystals with heightened nonlinear secondary optical susceptibility.



**Figure 1.8:** Example of banana-shaped liquid crystal

### 1.3.2 Lyotropic liquid crystals:

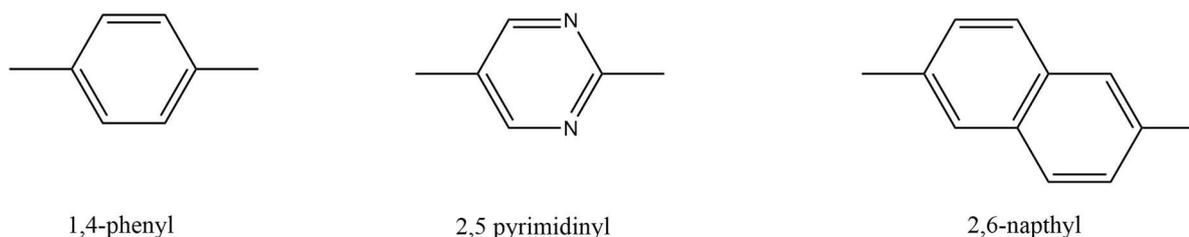
Amphiphilic molecules comprise the liquid crystalline phase of lyotropic materials [37]. The molecules are distinguished by a nonpolar tail and a hydrophilic polar head. Hydrocarbon chains, whether saturated or unsaturated, are common hydrophobic groups. In the right solvent, they self-assemble to form micelles. There are three known types of phase structures for lyotropic liquid crystals. This encompasses the lamellar phase, hexagonal columnar phase, and cubic phase. According to a recent theory, cohesive forces and water affinity play a role in the production of distinct phases in lyotropic substances [38].

## 1.4. Impact of Chemical Composition on Mesophase Formation

### 1.4.1 Core region:

The core is mostly responsible for the molecular asymmetry needed for its mesogenicity and the relatively high melting point. The lateral substituent and the centers are joined by

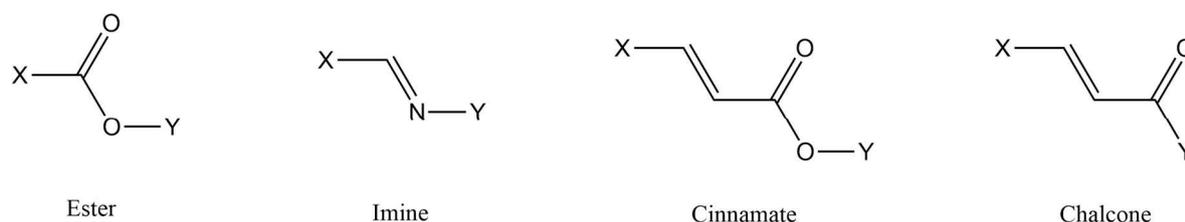
connecting groups. In general, calamitic liquid crystals contain alicyclic rings as well as aromatic rings like 1,4-phenyl, 2,5-pyrimidine, and 2,6-naphthalene. The melting point will often rise as the number of benzene rings increases. Moreover, the compound becomes increasingly mesogenic as the number of rings with linear connections grows. The structure of the ring changes somewhat when the  $-\text{CH}-$  group is altered out for an N atom, but the electrical characteristics shift is produced, altering the interaction.



**Figure 1.9:** Different core units

### 1.4.2 Linking groups:

Figure 1.10 shows the many connecting groups that are used in liquid crystal molecules. A structural element known as a connecting group joins the two halves of mesogens. The connectivity increases without changing its form, raises the molecular core's polarization anisotropy, and enhances the liquid crystal phase's stability. Due to its relative stability, ease of synthesis, and ability to create low-melt liquid crystals that are useful, the ester group is the most often employed connecting group in liquid crystals. A completely conjugated connecting group that can stretch molecules while maintaining linearity and enhancing longitudinal polarization is ethylene. Acetylene lengthens molecules while maintaining the core's stiffness, linearity, and polarization.



**Figure 1.10:** Different linking groups

### 1.4.3 Terminal groups:

The polarity of the terminal group in a molecule makes them significant. To maintain the molecule orientation, polar groups may generate strong intermolecular attraction forces. It was

discovered that the non-substituted mesogenic chemical had a less stable mesophase than the terminal substituted component. A specific kind of liquid crystal phase must occur, and this depends on the selection of end groups. According to Mayer and Saupe's theory [39], a compound's nematic-isotropic transition temperature is correlated with its polarity which is correlated with the side chain and how it affects intramolecular conjugation. There are terminal groups in smectic liquid crystals that decrease heat stability. The orientation required to stabilize the liquid crystal is a result of these chains. Pure nematic phases make up the majority of liquid crystals with medium chain lengths. While very long chains typically only feature smectic phases, longer carbon chains result in both smectic and nematic mesophases. Odd-numbered chains yield greater  $T_{N-I}$  values than even-numbered chains in terms of  $T_{N-I}$  trend values. The extra carbons that balances the trend and is known as the odd-even effect. The smectic tendency rises with end chain length, leading to the eventual elimination of the nematic phase [40].

#### 1.4.4 Lateral groups:

A lateral substituent is located usually away from the molecule's linear axis. Many distinct lateral substituents, such as F, Cl, CN, NO<sub>2</sub>, CH<sub>3</sub>, and CF<sub>3</sub>, are present in a wide variety of liquid crystal systems. While reducing lateral adhesion and separating molecules, lateral substitution can also increase molecular attraction. The lateral substitution broadens the molecule and causes a portion to rotate out of the plane [41]. Moreover, for the smectic phase rather than the nematic phase, the combined action of widening severely diminishes the temperature of the liquid crystal. The basic rule above does not apply to mesogens substituted by o-hydroxyl because intermolecular hydrogen bonds increase the molecule's overall polarizability [34]. Fluorine is the most often utilized lateral substituent. It is very polar, very tiny, and has a steric effects. Compared to fluorine substituents, chlorine substituents create greater dipoles. However, owing to its large size mesogenic material's stability, the chlorine substituent is not suited as it forms longer bonds with carbon. Regardless of the polarity of the substituents, the side group substituents generate a drop in  $T_{N-I}$  that is proportionate to their magnitude. The multilayer packing is broken by a big size but strengthened by a stronger polarity [1].

## 1.5. Identification of Liquid Crystals Phases

Due to their technical applications, several mesophases including mesomorphic substances are particularly significant. Therefore, it's critical to recognize different mesogens that a molecule exhibits.

The liquid crystal phases are identified and characterized using the primary techniques listed below:

### **Optical Polarizing Microscope:**

Optical polarising microscopy is the method of liquid crystal phase identification that is most frequently employed. This method exposes the unique optical texture of each separate liquid crystal phase. However, it can be challenging and time-consuming to identify liquid crystal phases using optical polarising microscopy.

### **Differential Scanning Calorimetry:**

By measuring the enthalpy change connected to a phase transition, DSC is always used for the conformation of different phases which was observed using POM. The degree of molecular ordering within a mesophase can be inferred from the level of enthalpy change, although this technique is unable to determine the kind of mesomorphic materials.

### **X-ray Analysis:**

X-ray analysis is the most effective method for identifying and categorizing mesophases. By mapping the locations of the molecules inside a phase, an X-ray examination of a liquid crystal can identify the phase structure and classification to which the specific phase belongs. However, aligned samples are required to maximize information.

### **Miscibility studies:**

Miscibility studies are a useful tool for identifying and classifying liquid crystal phases found in new substances. The substances with different phases are combined with a substance which have been identified as having certain mesophases (finally through X-ray analysis).

### **Neutron Scattering Studies:**

Typically, this technique is used to determine deuterated materials.

### **Nuclear Magnetic Resonance (NMR) studies:**

This technique is used to determine phases of lyotropic liquid crystals.

## 1.6. Applications of Liquid Crystals

### 1.6.1 Liquid Crystals Displays:

Numerous important scientific and engineering breakthroughs have been made in this subject, which has grown into a multibillion-dollar business. An LCD is essentially used to disperse light instead of producing light directly. Digital readout LCDs are found in a variety of equipment, including watches, calculators, mobile phones, flat TV panels, LCD projectors, and outdoor electronic advertising. Certain liquid crystal materials may have applications in the computer industry, including the development of new high-memory computer components.

### 1.6.2 Temperature Sensors:

There are several uses for liquid crystals as temperature sensors. The most widely used gadget relies on chiral nematic liquid crystals' ability to selectively reflect light. When white light is incident on a chiral nematic material, the angle of view and the chiral nematic pitch dictate the wavelength of the light that is reflected. Therefore, in white light, certain chiral nematic liquid crystals look highly colored. A chiral nematics pitch is temperature-dependent, hence temperature variations affect the color that is observed. When different combinations are used properly, a large range of response options for temperature sensors can be produced.

### 1.6.3 Polymer-Dispersed Liquid Crystals (PDLCs):

Polymer-dispersed liquid crystals, or PDLCs, are a relatively new family of materials with a wide range of potential uses, including projection screens and switchable windows. These materials are essentially polymers and liquid crystals applied together. The display industry is doing a lot of research on these materials. Particle-dispersed liquid crystals are the building blocks of phase-change memory liquids (PDLCs). The resultant substance resembles a "Swiss cheese" polymer, with the gaps filled up by liquid crystal droplets. The material's distinct behaviour is caused by these microscopic droplets, which are only a few microns in diameter for practical use. Light intensity can be adjusted by adjusting the orientation of liquid crystal molecules in the presence of an electric field. Polymer-dispersed liquid crystals have the potential to be used in light shutters and displays, among other electro-optic applications. An extremely thin layer of indium tin oxide (ITO), a conducting substance, is applied to the plastic substrates.

The primary means of light transmission through a phase-change lens compactor (PDLC) window is scattering, which is contingent upon the disparity in refractive index between the droplets and their surroundings. The surrounding is primarily made up of other droplets therefore, the relative orientation plays a crucial role. Because of their anisotropic nature, the droplets parallel to the direct index of refraction differ from their perpendicular index.

The random array of droplet orientation in the field OFF produces considerable scattering and notable disparities in indices. At this point, the cell appears translucent. However, the direction of each droplet aligns with the field when a voltage is applied. The cell now appears transparent and the refractive index variation between adjacent droplets is minimal.

### 1.6.4 Medical Applications:

It makes it easier to identify nervous system injury. When a nerve is injured, the area where the nerve is distributed has an increase in temperature, which eventually cools down. The temperature variation anomaly is still limited to the region where the damaged nerve is distributed. It is possible to employ liquid crystalline materials as a carrier for a controlled medication delivery system [43, 44]. These materials can be used in gynecology. Cholesteric materials are used as lie detectors in psychology.

### 1.6.4 Cosmetics:

A significant portion of cosmetic products are emulsions, which enable hydrophilic and lipophilic substances in the necessary dosages. An emulsion material also has the benefit of having the most user-friendly texture and look, which makes application easier. They can be made into liquids, creams, or even extremely sprayable substances [45]. The following are the benefits of liquid crystals for emulsion.

#### **Stability:**

Coalescence is inhibited by the multilayers surrounding the oil droplets emulsion stability. When oil droplets combine, the emulsion fractures. This coalescence barrier contributes to the emulsion's improved stability.

#### **Prolonged hydration:**

Water layers are found in lamellar liquid crystalline and gel networks. This type of water has a longer-lasting moisturizing impact on the skin, which is important for drug absorption and is less likely to evaporate when applied.

### **Controlled Drug Delivery:**

This kind of medicine is not allowed to be released quickly. The layered structure is responsible for this, as it lessens the drug's interfacial transit as it dissolves in the oil droplets. Under polarised light, microscopic inspection reveals the extraordinarily thick liquid crystalline lamellar layer surrounding the oil droplets.

### **Optical Imaging:**

Optical recording and imaging is a use of liquid crystals that is just now being investigated. This approach involves sandwiching a liquid crystal cell between two photoconductor layers. The photoconductor receives light, which raises the material's conductivity. As a result, the liquid crystal develops an electric field in proportion to the light's intensity. An electrode can convey the electric pattern, allowing for the recording of the image. Currently under development, this technology represents one of the most promising fields of study for liquid crystals.

## **1.7. Other Uses of Mesogenic Materials**

High-strength fibers can be produced by processing polymer liquid crystals. During the production process, the main chain polymer liquid crystals spontaneous orientational order can be "frozen in," producing significantly stronger fibers than if the polymer chains remained unoriented. The most well-known example is the polyamide Kevlar.

In chromatographic applications, liquid crystals can be utilized to create an anisotropic media that facilitates the separation of related molecules.

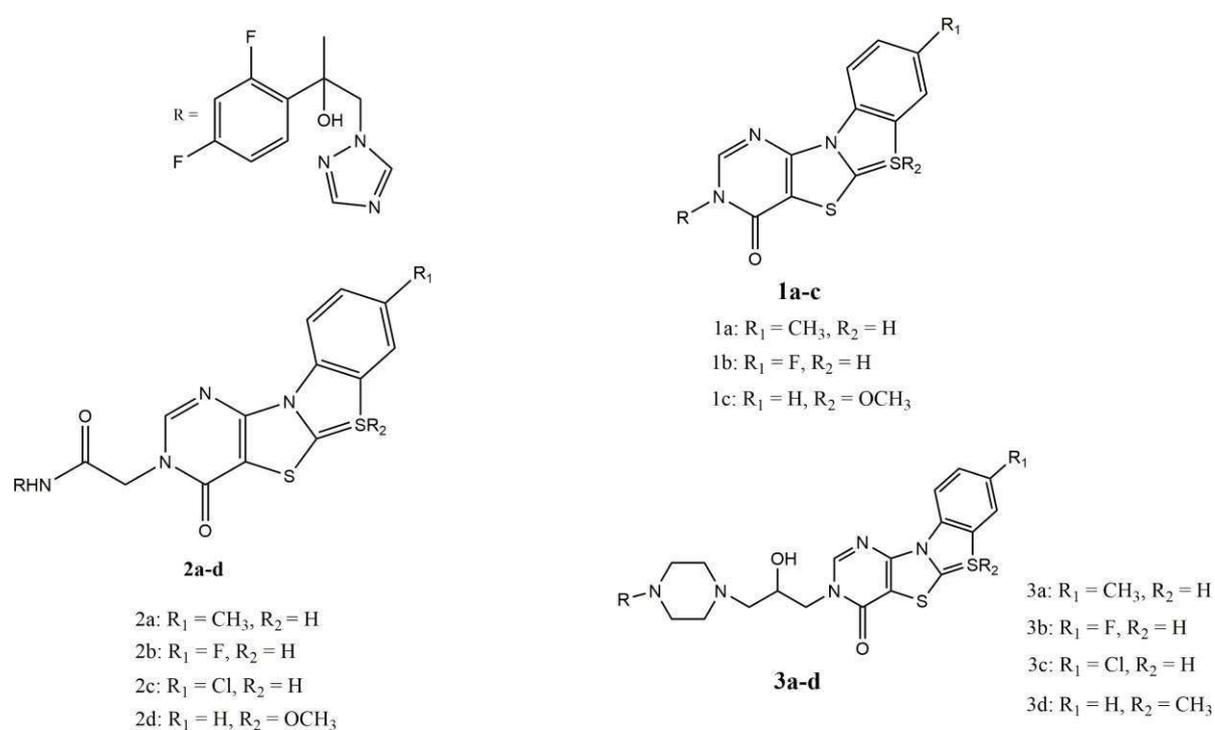
For some spectral uses, liquid crystals can function as anisotropic solvents. NMR spectroscopy measures the anisotropic chemical shifts and dipolar and quadrupolar splitting of chemicals dissolved in a nematic liquid crystal by the analysis of their NMR spectra.

Cholesteric liquid crystals sensitivity to temperature and pressure is exploited to create some quite intriguing toys and promotional items. By detecting colour changes to the extent of approximately 1 ppm, cholesteric liquid crystals can be employed as an analytical technique to identify the presence of very minute amounts of gases or vapours.

## **1.8. Biologically active compounds**

Due to their many important biological and medicinal applications, heterocyclic compounds have attracted a lot of research in the field of science. Heterocyclic compounds have garnered

significant attention in research because of their long synthetic history and practical applications. They bridge the gap between biology and chemistry, where so much scientific research and application takes place, and are present in more than 90% of innovative medications. Additionally, heterocycles are used in a variety of disciplines, such as biochemistry and medicinal chemistry. Applications for heterocyclic compounds are mostly found in pharmaceuticals, agrochemicals, and veterinary products. A new phase of potential bioactive heterocycles with potential antifungal, anti-inflammatory, antibacterial, antiviral, antioxidant, anticonvulsant, anthelmintic, antipyretic, anti-allergic, anti-histamine, herbicidal, anticancer, antihypertensive, and anti-leprosy properties is covered in our review, which also covers the majority of recently synthesized bioactive heterocycles.

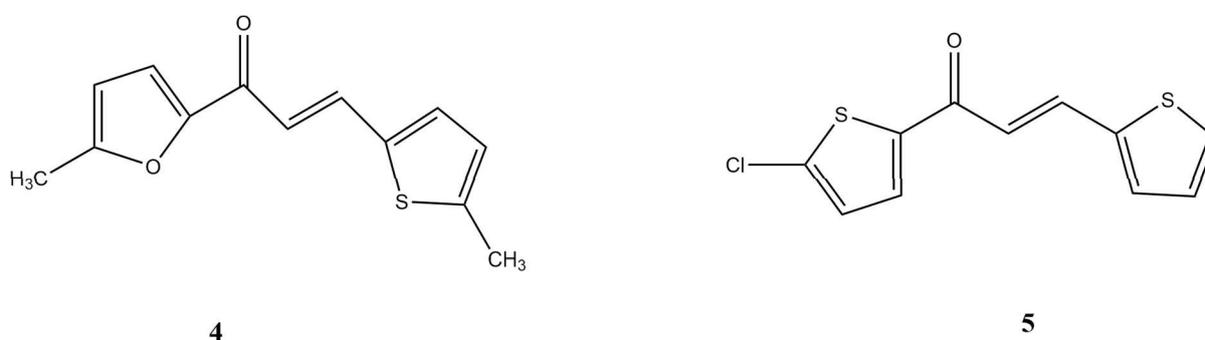


**Figure 1.11:** Structures of thiazole [4, 5-d] pyrimidines derivatives with (1*H*-1,2,4)-triazol.

The most prevalent hetero-atoms are sulphur, nitrogen, and oxygen; however, heterocyclic rings containing other hetero-atoms, such as phosphorus, iron, magnesium, selenium, and so on, are also frequently found [46-48]. The most significant traditional subfield of organic chemistry is heterocyclic chemistry, which is gaining attention in research due to its industrial, antimicrobial, and medical uses [49-51]. Numerous heterocyclic compounds, such as analogs of triazine, have been used as an anti-inflammatory, urinary antiseptic, and therapeutic agent in the treatment of a wide range of illnesses [52]. Benzimidazole derivatives have shown

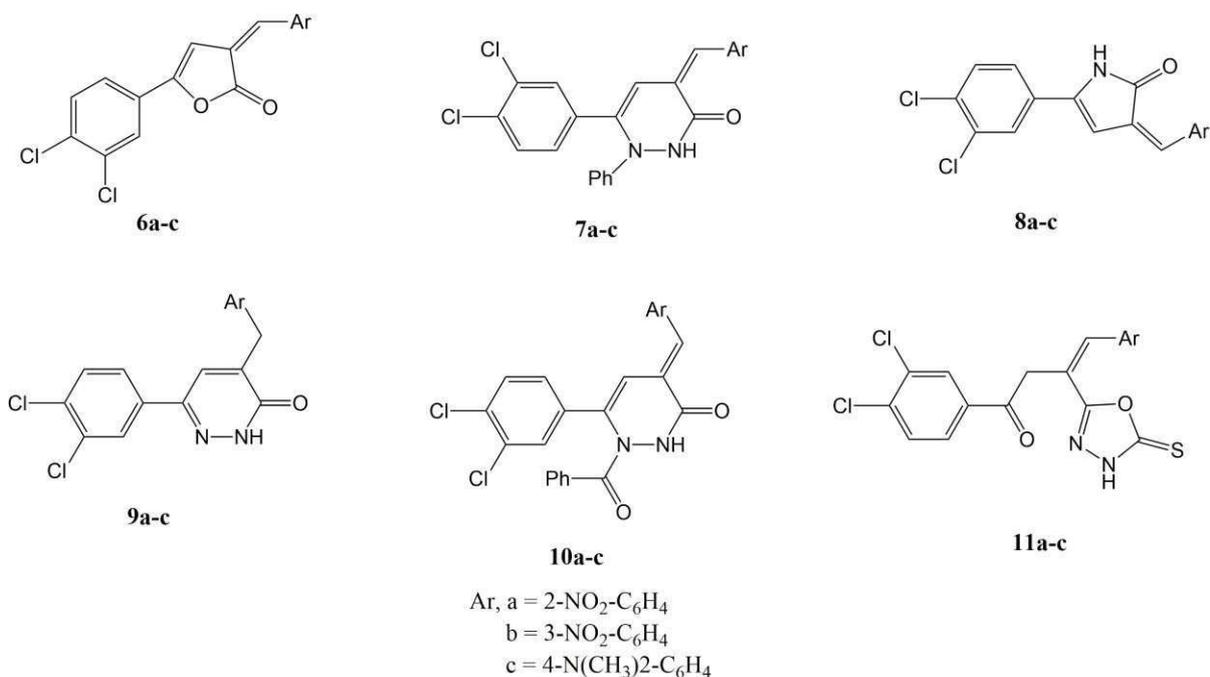
antibacterial, antifungal, antiviral, and anthelmintic activities [53–56]. Most pharmaceutical drugs are composed of heterocyclic molecules. Some of the most common heterocycles are vitamins and precursors including pyridoxine, riboflavin, thiamine, biotin, folic acid, and B12, as well as amino acids like histidine, tryptophan, and proline [57–59].

Using fluconazole as the positive control, S.V. Blokhina *et al.* [60] synthesized novel thiazole [4,5-d] pyrimidine derivatives and (1*H*-1,2,4)-triazole (Figure 1.11) to study their antifungal activity against various cultures in-vitro activity. Fluconazole was used as the positive control at different doses when L.S. Ming *et al.* [61] synthesized thiophene-based heterocyclic chalcones that demonstrated antifungal efficacy against fungus (Figure 1.12).

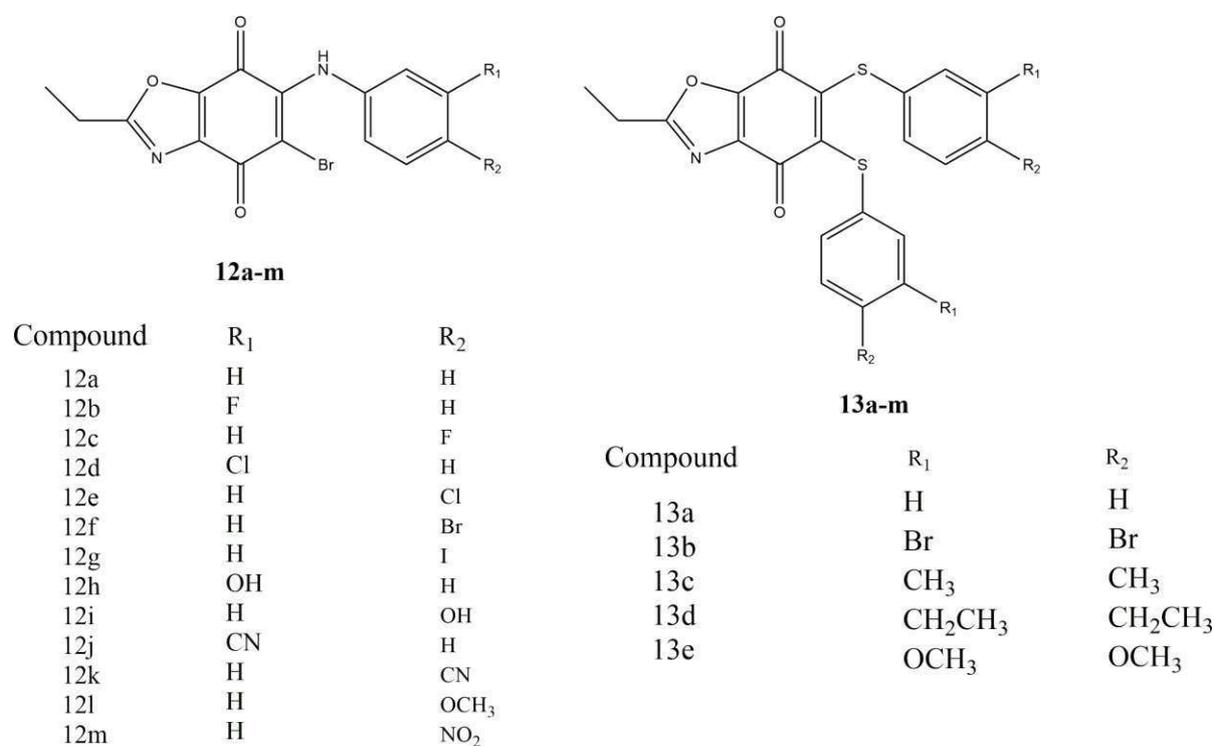


**Figure 1.12:** Thiophene-based heterocyclic chalcones

C.K. Ryu and others [62] produced heterocycles of benzo-[d]oxazole-4,7-iones and evaluated their antifungal effectiveness against harmful fungi by comparing them to 5-fluorocytosine, a widely used standard drug (Figure 1.14). The anti-inflammatory properties of all the synthesized drugs were tested by E. I. Hameed *et al.* [63] who synthesized various novel heterocyclic derivatives of furan, pyrrole, 4-oxabutanamide, 1-phenyl-1,4-dihydropyridazin-3(2*H*)-one, 4-oxo-butanhydrazide, 1*H*-pyridazin-6-one, 3-(3,4-dichlorophenyl)-1*H*-pyridazin-6-one, 3-(2-thioxo-4,5-dihydro-1,3,4-oxadiazol-5-yl)but-3-en-1-one (Figure 1.13).

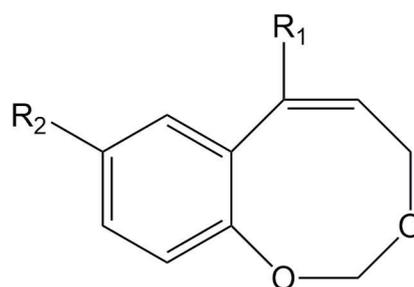


**Figure 1.13:** Structure of furan, pyrrole, 4-oxabutanamide, 1-phenyl-1,4-dihydropyridazin-3(2*H*)-one, 4-oxo-butanehydrazide, 1*H*-pyridazin-6-one, 3-(3,4-dichlorophenyl)-1*H*-pyridazin-6-one, 3-(2-thioxo-4,5-dihydro-1,3,4-oxadiazol-5-yl)but-3-en-1-one.



**Figure 1.14:** Structures of benzo-[d]oxazole-4, 7-iones heterocycles

A class of compounds known as antibacterial chemicals works against harmful germs by preventing their growth. The chemical structure of antibiotics contains heterocyclic aromatic molecules, such as those derived from lactams. Many substances appear to possess all of this action, and testing them against a variety of bacteria has produced encouraging findings for the treatment of several common ailments. To explore the antibacterial properties of aerobic bacteria, Y. F. Mustafa *et al.* [64] synthesized novel heterocycles of coumacine derivatives, which were then screened using metronidazole for anti-anaerobic research of coumarin and its derivatives as well as ciprofloxacin as a positive control (Figure 1.15).



14a-c

Compound	R <sub>1</sub>	R <sub>2</sub>
a. Coumarin	H	H
b. Coumarin I	CH <sub>3</sub>	CH <sub>3</sub>
c. Coumarin II	Phenyl	CH <sub>3</sub>

Figure 1.15: Structure of coumarin derivatives

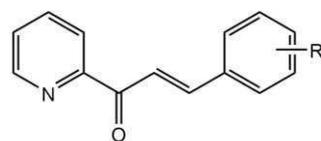
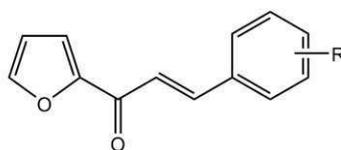
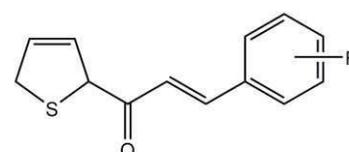
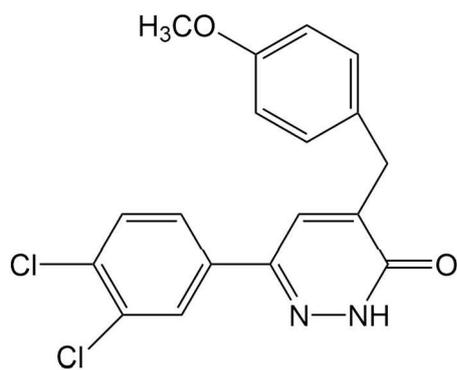
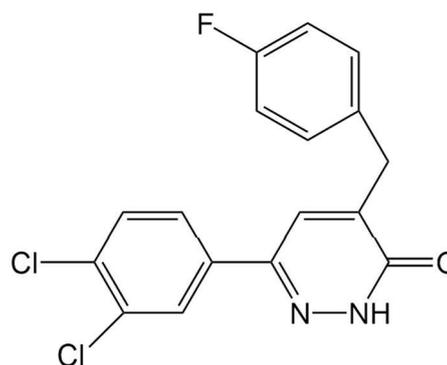

 where R = pyridine-2-yl  
 15a-g

 where R = thiophene-2-yl  
 16a-g

 R = furan-2-yl  
 17a-g

Figure 1.16: Biologically active chalcone derivatives

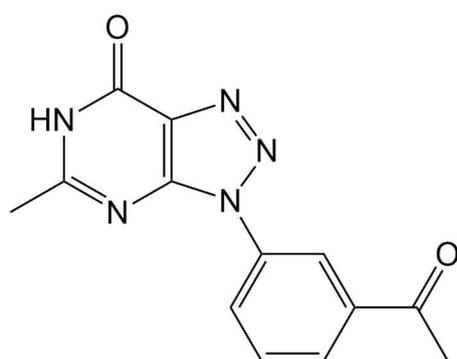


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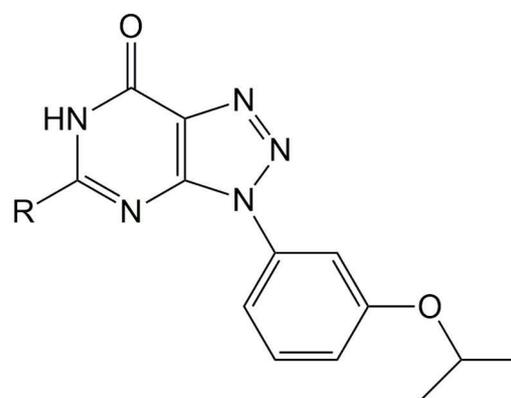


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**Figure 1.17:** Biologically active pyridazinones derivatives



20

where R = CH<sub>3</sub> 21

**Figure 1.18:** Biologically active [1,2,3] triazole[4,5-d]pyrimidine-7(6H)-ones

The derivatives of heterocyclic chalcones were created by T. D. Tran *et al.* [65] using the Claisen-Schmidt condensation process. The methicillin-sensitivity of every chemical was tested against bacteria that was obtained from a human sample (Figure 1.16). Pyridazinones were synthesized by A. E. Hameed *et al.* [66] and their antiviral efficacy against rotavirus and adenovirus was evaluated (Figure 1.17). Triazolo[4,5-d]pyrimidin-7(6H)-ones were synthesized by A. Gigante *et al.* [67] and their antiviral effects against the chikungunya virus (CHIKV) were demonstrated (Figure 1.18).

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