

Abstract of the  
Thesis entitled

**Synthesis, Characterization and Applications  
of Cholesterol/Heterocyclic based  
Mesogenic Compounds**

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This thesis presents the synthesis and comprehensive characterization of novel liquid crystalline compounds, incorporating cholesterol and various heterocyclic moieties with different functional groups. These compounds were designed to explore new structural varieties and enhance performance characteristics for diverse applications. The study encompasses the synthesis of homologous Schiff's bases, azo-biphenyl derivatives and heterocyclic derivatives, and other compounds each exhibiting unique mesomorphic properties.

**Chapter 1** provides an introduction to the realm of liquid crystals, including a historical overview, classification and the relationship between molecular structure and mesomorphic properties. It sets the stage for understanding the broad spectrum of applications and the importance of molecular design in tailoring liquid crystal behaviour.

**Chapter 2** details the synthesis of twenty-six new mesogenic Schiff's base derivatives (1a-m and 1' a-m) by condensing 4-n-alkoxy aniline with 4-formyl phenyl cholesteryl carbonate and 4-formyl 3-methoxy phenyl cholesteryl carbonate. All the compounds were characterised using elemental analysis, FT-IR,  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$ . In order to study the liquid crystalline behaviour of the synthesised compounds, optical texture studies were carried out using polarising optical microscope in heating and cooling cycles. The derivatives showed a variety of mesophases, including chiral nematic ( $\text{N}^*$ ), twist grain boundary-A ( $\text{TGB}_\text{A}$ ), smectic A ( $\text{SmA}$ ), and chiral smectic C ( $\text{SmC}^*$ ) phases. The thermal behaviour was determined using a differential scanning calorimeter and thermogravimetric analysis. All the synthesised compounds are UV-active and show photoluminescence in the blue emission region with good quantum yield. The effect of lateral methoxy substitution is examined, revealing a reduction in thermal as well as mesophase stability. DFT calculations provide insights into theoretical chemical reactivity.

**Chapter 3** outlines the systematic design and synthesis of thirteen new liquid crystalline derivatives with cholesteryl group and biphenyl moiety interconnected with azo-carbonate linking groups and terminal alkoxy chains. All the compounds were characterised using elemental analysis and spectroscopic techniques such as FT-IR,  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$ . The mesomorphic properties of all the compounds were investigated in heating and cooling cycles using a crossed polarising optical microscopy (POM). The derivatives displayed a wide variety of mesophases, including chiral nematic ( $\text{N}^*$ ), twist grain boundary-A ( $\text{TGB}_\text{A}$ ) and smectic A ( $\text{SmA}$ ) mesophases. The isotropic temperature of all the compounds within the homologous series seems to decline with the increase in carbon numbers on flexible chains.

The thermal behaviour of all the synthesised compounds was checked using differential scanning calorimetry and thermogravimetric analysis. The photo responsive behaviour of the synthesised compounds was well examined by UV study. The radical scavenging activity of the synthesised mesogenic derivatives were also evaluated using the DPPH assay. Theoretical chemical reactivity studies using Density Functional Theory focused on analyzing Frontier Molecular Orbitals and Molecular Electrostatic Potential mapping to identify energy gaps and regions of varying electron density.

**Chapter 4** describes the design and synthesis of thirteen new homologues Schiff's base derivatives were synthesised by condensing 4-formyl phenyl cholesteryl carbonate with 5-(4'-n-alkoxy phenyl)-2-amino-1,3,4-thiadiazole. All the synthesised derivatives were characterised using elemental analysis, FT-IR,  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$ . Optical texture studies were carried out using a polarising optical microscope in heating and cooling cycles to examine the liquid crystalline behaviour of the synthesised compounds. The derivatives displayed a variety of mesophases, including chiral nematic ( $\text{N}^*$ ), twist grain boundary-A ( $\text{TGB}_A$ ), smectic A ( $\text{SmA}$ ) and chiral smectic C ( $\text{SmC}^*$ ) phases. The isotropic temperature of all the compounds within the homologous series seems to decline with the increase in carbon numbers on flexible chains. The thermal behaviour of all the synthesised compounds was checked using differential scanning calorimetry and thermogravimetric analysis. All the synthesised compounds are UV-active and exhibit photoluminescence in the blue emission band with a remarkable quantum yield. The radical-scavenging activity of the synthesised mesogenic derivatives was also evaluated using the DPPH assay. Theoretical studies further elucidate their electronic structure and potential applications.

**Chapter 5** reports the synthesis of homologous series of non-symmetric 1,3,4-oxadiazole liquid crystal compounds consisting azomethine and ester linkages. Thirteen new derivatives were synthesized by condensing 5-(4'-n-alkoxy phenyl)-2-amino-1,3,4-oxadiazole with 4-methoxybenzoyloxy benzaldehydes. All the synthesised compounds were confirmed by elemental analysis and characterized using various spectral techniques such as FT-IR,  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$ . In order to investigate the different properties of liquid crystals the optical texture studies were carried out using optical polarising microscope. The synthesized derivatives show enantiotropic mesophases including nematic (N), smectic A ( $\text{SmA}$ ) and smectic C ( $\text{SmC}$ ) phases. The isotropic transition temperature of all the compounds decreases with the increasing terminal carbon chain length. The thermal behaviour was determined using a differential scanning calorimeter and thermogravimetric analysis. Synthesised compounds

are UV-active and show photoluminescence in the blue emission region with remarkable quantum yield. The radical scavenging activity of the synthesised mesogenic derivatives were also evaluated using the DPPH assay. Also, DFT studies have been carried out including frontier MOs and MEP analysis.

**Chapter 6** investigates the synthesis of four new Schiff's bases by condensing 2-amino-1,3-thiazole with substituted formyl phenyl cholesteryl carbonates. The compounds were thoroughly characterized using elemental analysis and spectral techniques such as  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and FT-IR. Optical texture investigations were conducted on the synthesized compounds to analyze their liquid crystalline behaviour using an optical polarizing microscope in heating and cooling cycles. Among all the derivatives, only compound 7a exhibited liquid crystalline behaviour, showing chiral nematic ( $\text{N}^*$ ) mesophase. The thermal properties were analyzed using a differential scanning calorimeter as well as thermogravimetric analysis. The synthesized compounds were tested in vitro for antibacterial activity towards gram-positive (*Staphylococcus aureus*) and gram-negative (*Escherichia coli*) bacteria. The compounds were also examined for their inhibitory effects on *Aspergillus niger* and *Candida albicans* strains of fungus. The antioxidant potential of all the compounds were assessed using the DPPH test. All synthesized derivatives are UV-active and display photoluminescence within the blue emission range. In silico predictions were made for drug likeness and bioactivity scores as well. Moreover, DFT calculations were discussed for all the compounds.

**Chapter 7** concludes with a comprehensive summary of all the work presented and derives main conclusions from the investigations conducted. As discussed, this research probes into the fascinating area of liquid crystals, focusing on cholesterol-based derivatives and other liquid crystals. These compounds, combining liquid and crystalline properties, offer unique mesophases and applications. Emphasizing molecular design, synthesis and characterization, the study systematically explores homologous series variations. Characterization techniques, including spectroscopy and microscopy, provide insights into properties and potential applications. Liquid crystals, with adaptability beyond laboratories, contribute to diverse fields from display technologies to drug delivery systems

The outcomes of this research suggest that the synthesized liquid crystal materials exhibit promising properties for diverse applications. This thesis contributes to the understanding of structure-property relationships in liquid crystal materials and provides a basis for the development of novel compounds with enhanced properties and applications.