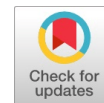


# Synthesis and Physicochemical Properties of Coumarin Derivatives as Antimicrobial Agents

Manisha, Anita Singh, Pravin K Singh



**Abstract:** A series of new coumarine Schiff base derivatives has been designed using in silico methods and synthesised as potential antimicrobial agents. Furthermore, the compounds were evaluated for their antibacterial and antifungal properties. In silico results indicate that all the compounds adhere to the Lipinski rule of five.

**Keywords:** Schiff base, ADME, MIC, Molinspiration, Chem Draw, Lipinski's Rule

## Abbreviations:

FIC: Fractional Inhibitory Concentration

MIC: Minimum Inhibitory Concentration

TLC: Thin-Layer Chromatography

PSA: Polar Surface Area

TPSA: Total Polar Surface Area

## I. INTRODUCTION

Microbes are a significant cause of deadly diseases, and their widespread transmission poses an escalating threat to human health [1]. Effectively treating these severe infections and eliminating antimicrobial resistance [2] requires the deployment of novel antimicrobial agents, a crucial area of ongoing scientific research. Utilizing potent chemotherapeutic agents can shorten treatment durations and reduce the emergence of new resistant strains. Exploring appropriate combinations of existing and novel antimicrobial candidates as drug regimens could help eradicate the pressing issue of drug resistance [3]. Extensive research into antimicrobial agents has revealed protein synthesis as the most promising target among several for developing powerful drugs [4]. Despite considerable progress in antibacterial therapy and the availability of inhibitors against drug-resistant Gram-positive and Gram-negative bacterial strains, a critical need remains for new drugs or drug regimens with optimal safety profiles to overcome drug resistance [5]. Similarly, life-threatening ailments caused by pathogenic fungi are a regular challenge, particularly in immunocompromised patients.

Although fungal infections are widespread, treatment options are limited, making the research and development of novel antifungal drugs essential at present [6]. Schiff bases, formed by the condensation of primary amines with carbonyl groups, have recently garnered significant attention [7] due to their diverse biological and industrial applications. The imine functional group, specifically the azomethine moiety with its sp<sup>2</sup> hybridized nitrogen atom bearing a lone pair of electrons, enables these compounds to interact uniquely with nucleophiles and electrophiles. This allows them to perform various roles, including antibacterial, anticancer, antifungal, and radical scavenging activities, and to function as enzymatic intermediates or inhibitors in biochemical processes. The formyl functional group within the 2H-chromen-2-one ring, also known as the coumarin ring, is key to extending its reactivity. This functionality facilitates the formation of Schiff bases of 2H-chromen-2-one, where the formyl group can be selectively attached to either the benzene ring or the 2H-pyran-2-one ring at various positions within the coumarin structure [8]. The inherent planarity of the fused lactone ring enables coumarin to engage in non-covalent interactions with biomolecules, such as proteins and DNA, contributing to its diverse range of biological activities [9]. Furthermore, recent modifications of benzopyrone framework-based coumarins have led to the development of several derivatives with remarkable antibacterial efficacy. Coumarin exhibits a broad spectrum of pharmacological activities, including antibacterial [10], antioxidant [11], anti-inflammatory [12], anticancer, and antifungal [13] properties. Given the significant therapeutic potential of coumarin and its derivatives, these compounds continue to attract substantial scientific interest for their diverse biological effects [14]. Notably, certain coumarin-based antibiotics, such as novobiocin, clorobiocin, and coumermycin A1, have achieved clinical success in combating acute infections, fueling further exploration for new coumarin-based antibacterial agents.

Our research involved assessing the physicochemical and pharmaceutical properties of the designed molecules using various in silico techniques. The collected data were compiled and analyzed for further investigation. To evaluate antibacterial activity, the Minimum Inhibitory Concentration (MIC) value of the synthesised compounds was determined [15]. A combination approach was also employed to calculate the \*Fractional Inhibitory Concentration (FIC), which helped in studying the synergistic effects of the tested compounds and standard references [16]. This approach may lead to the development of potential drug regimens against human pathogenic bacteria. Similarly, antifungal activities were examined using both the zone inhibition method and the serial broth microdilution method [17].

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## II. EXPERIMENTAL

### A. Design, Physicochemical Descriptors and ADME Properties of Schiff Base of Coumarin Derivative

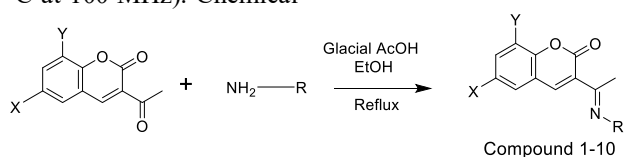
Using Molinspiration and ChemDraw software, some physically significant descriptors and pharmaceutically relevant properties of compounds, such as molecular weight, H-bond donors, H-bond acceptors, logP, rotatable bonds, and TPSA, have been analysed based on Lipinski's rule of five. ADME properties, such as aqueous solubility (LogS), skin permeability (Log Kp), synthetic accessibility scores, and Absorption (%ABS), were calculated using DS 2.5 software.

## III. CHEMISTRY

All chemicals and reagents were purchased from Sigma-Aldrich Chemical Company, USA, and E. Merck India Ltd, India. All reactions were performed in oven-dried apparatus using dried and distilled solvents. The progress of the reaction was monitored by thin-layer chromatography (TLC) using silica gel 60F254 aluminium sheets, and visualised under ultraviolet light at 254 nm. Synthesized compounds were purified by column chromatography by using silica gel (100–200 mesh). Melting points recorded on an electrothermal apparatus using open capillary tubes are uncorrected. NMR spectra were recorded on a BRUKER AV400 spectrometer (Bruker Co., Fällanden, Switzerland) in DMSO-d<sub>6</sub> (<sup>1</sup>H at 400 MHz and <sup>13</sup>C at 100 MHz). Chemical

shifts (δ) are expressed in parts per million (ppm) and J (coupling constant) values in Hz. Multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). The elemental analyses were performed on Perkin-Elmer 240-C analysis equipment.

For the synthesis of Schiff base, two coumarin derivatives, viz. 3-acetyl-6-chloro-2H-chromen-2-one, 3-acetyl-8-methoxy-2H-chromen-2-one and commercially available different types of aromatic amines, viz. benzo[d]oxazol-6-amine, 2,3-dihydrobenzo[b][1,4]dioxin-6-amine, benzo[d]oxazol-2-amine, 1-methyl-6-phenyl-1H-benzo[d]imidazol-2-amine, 21,6-dimethyl-1H-imidazo[4,5-b]pyridin-2-amine have been used. For the synthesis of the coumarin Schiff base, the compound was treated with commercially available different aromatic amines (1:1) in ethanol (30 mL) containing a few drops of glacial acetic acid. The resulting reaction mixture was heated at 40°–50°C for 3–4 hours. TLC checked the progress of the reaction. After the reaction was completed, the mixture was cooled to room temperature, concentrated, and then poured into ice-cold water. It was subsequently basified with 2 M NaOH (pH 10), resulting in the formation of a precipitate. The precipitate was filtered, washed with water, and dried over CaCl<sub>2</sub> in the vacuum chamber to obtain the crude product. The product was then purified by column chromatography and finally crystallized using ethanol. The characterisation was performed using <sup>1</sup>H NMR, mass spectrometry, and elemental analysis techniques.



Compound	X	Y	R	Structure
1	Cl	H		
2	Cl	H		
3	Cl	H		
4	Cl	H		
5	Cl	H		

6	H	OCH <sub>3</sub>		
7	H	OCH <sub>3</sub>		
8	H	OCH <sub>3</sub>		
9	H	OCH <sub>3</sub>		
10	H	OCH <sub>3</sub>		

**(E)-3-(1-(benzo[d]oxazol-6-ylimino) ethyl)-6-chloro-2H-chromen-2-one**

White colour solid, M.P. 206 °C, yield 35 %. <sup>1</sup>H NMR: δ 2.30 (3H, s), 7.37-7.59 (4H, 7.43 (dd, *J* = 6.0, 1.7 Hz), 7.46 (dd, *J* = 8.0, 0.4 Hz), 7.53 (dd, *J* = 8.0, 1.7 Hz), 7.54 (dt, *J* = 1.7, 0.4 Hz)), 7.84 (1H, dd, *J* = 1.7, 0.4 Hz), 8.12-8.28 (2H, 8.18 (dt, *J* = 6.0, 0.4 Hz), 8.23 (t, *J* = 0.4 Hz)), 8.36 (1H, s) <sup>13</sup>C NMR: δ 24.6 (1C, s), 110.3 (1C, s), 114.8 (1C, s), 116.0 (1C, s), 117.1 (1C, s), 117.5 (1C, s), 120.4 (1C, s), 121.1 (1C, s), 133.1 (1C, s), 133.5 (1C, s), 140.1 (1C, s), 147.3 (1C, s), 147.6 (1C, s), 152.6 (1C, s), 154.4 (1C, s), 154.7 (1C, s), 159.1 (1C, s), 160.8 (1C, s).

**(E)-6-chloro-3-(1-((2,3-dihydrobenzo[b][1,4]dioxin-6-yl)imino)ethyl)-2H-chromen-2-one**

Light brown colour solid, M.P. 195-201 °C, yield 32 %. <sup>1</sup>H NMR: δ 2.29 (3H, s), 4.21 (2H, ddd, *J* = 13.7, 7.0, 1.8 Hz), 4.50 (2H, ddd, *J* = 17.8, 7.0, 1.8 Hz), 6.77-6.99 (3H, 6.84 (dd, *J* = 8.6, 0.5 Hz), 6.88 (dd, *J* = 8.6, 1.3 Hz), 6.94 (dd, *J* = 1.3, 0.5 Hz)), 7.35-7.52 (2H, 7.41 (dd, *J* = 8.0, 1.6 Hz), 7.46 (dd, *J* = 8.0, 0.5 Hz)), 7.89 (1H, dd, *J* = 1.6, 0.5 Hz), 8.11 (1H, s). <sup>13</sup>C NMR: δ 24.6 (1C, s), 64.2-64.3 (2C, 64.2 (s), 64.2 (s)), 98.2 (1C, s), 114.8 (1C, s), 116.0 (1C, s), 117.3 (1C, s), 117.5 (1C, s), 120.4 (1C, s), 123.8 (1C, s), 132.6 (1C, s), 133.1 (1C, s), 133.5 (1C, s), 143.3 (1C, s), 147.3 (1C, s), 149.4 (1C, s), 154.4 (1C, s), 159.1 (1C, s), 160.8

**(E)-3-(1-(benzo[d]oxazol-2-ylimino) ethyl)-6-chloro-2H-chromen-2-one**

Cream colour solid, M.P. 217 °C (208 °C lit), yield 57 %. <sup>1</sup>H NMR: δ 2.30 (3H, s), 7.36-7.53 (2H, 7.43 (ddd, *J* = 7.7, 7.5, 1.5 Hz), 7.47 (dd, *J* = 8.2, 0.4 Hz)), 7.54-7.77 (4H, 7.62 (ddd, *J* = 8.0, 7.5, 1.7 Hz), 7.62 (dd, *J* = 1.6, 0.4 Hz), 7.68 (ddd, *J* = 8.0, 1.5, 0.5 Hz), 7.70 (dd, *J* = 8.2, 1.6 Hz)), 8.04 (1H, ddd, *J* = 7.7, 1.7, 0.5 Hz), 8.66 (1H, s). <sup>13</sup>C NMR: δ 24.6 (1C, s), 109.3 (1C, s), 114.8 (1C, s), 116.0-116.0 (2C, 116.0 (s), 116.0 (s)), 117.5 (1C, s), 120.4 (1C, s), 124.4 (1C, s), 125.1 (1C, s), 133.1 (1C, s), 133.5 (1C, s), 143.4 (1C, s), 147.3 (1C, s), 149.2 (1C, s), 154.4 (1C, s), 159.1 (1C, s), 160.8 (1C, s), 169.5 (1C, s).

**(E)-6-chloro-3-(1-((1-methyl-6-phenyl-1H-benzo[d]imidazol-2-yl)imino)ethyl)-2H-chromen-2-one**

Light green colour solid, M.P. 191 °C, yield 38 %. <sup>1</sup>H NMR: δ 2.32 (3H, s), 4.03 (3H, s), 7.35-7.79 (9H, 7.41 (dd, *J* = 8.3, 0.4 Hz), 7.51 (tdd, *J* = 5.9, 1.8, 1.6 Hz), 7.53 (dd, *J* = 1.8, 0.5 Hz), 7.57 (dd, *J* = 8.3, 1.7 Hz), 7.63 (dddd, *J* = 7.3, 5.9, 1.9, 0.5 Hz), 7.68 (dd, *J* = 1.7, 0.4 Hz), 7.73 (dddd, *J* = 7.3, 1.7, 1.2, 0.5 Hz)), 7.94 (1H, dd, *J* = 5.1, 1.8 Hz), 8.10 (1H, dd, *J* = 5.1, 0.5 Hz), 8.38 (1H, s). <sup>13</sup>C NMR: δ 21.4 (1C, s), 24.6 (1C, s), 110.3 (1C, s), 114.8 (1C, s), 116.0 (1C, s), 117.1 (1C, s), 117.5 (1C, s), 120.4 (1C, s), 124.8 (1C, s), 126.9 (2C, s), 128.2 (1C, s), 128.9 (2C, s), 133.1 (1C, s), 133.5 (1C, s), 134.2 (1C, s), 138.1-138.2 (2C, 138.2 (s), 138.2 (s)), 139.9 (1C, s), 140.3 (1C, s), 147.3 (1C, s), 154.4 (1C, s), 159.1 (1C, s), 160.8 (1C, s)

## (E)-6-chloro-3-(1-((1,6-dimethyl-1H-imidazo[4,5-b]pyridin-2-yl)imino)ethyl)-2H-chromen-2-one

White colour solid, M.P. 176-180 °C. <sup>1</sup>H NMR: δ 2.17 (3H, s), 2.34 (3H, s), 4.02 (3H, s), 7.41-7.67 (3H, 7.47 (dd, *J* = 8.2, 0.4 Hz), 7.56 (dd, *J* = 1.6, 0.4 Hz), 7.61 (dd, *J* = 8.2, 1.6 Hz)), 8.11 (1H, d, *J* = 1.7 Hz), 8.50-8.67 (2H, 8.55 (s), 8.62 (d, *J* = 1.7 Hz)). <sup>13</sup>C NMR: δ 18.4 (1C, s), 24.6 (1C, s), 32.9 (1C, s), 114.8 (1C, s), 116.0 (1C, s), 117.5 (1C, s), 119.5 (1C, s), 120.4 (1C, s), 130.4 (1C, s), 133.1 (1C, s), 133.5 (1C, s), 139.9 (1C, s), 144.6 (1C, s), 147.3 (1C, s), 151.1 (1C, s), 154.4 (1C, s), 159.1 (1C, s), 160.8 (1C, s), 164.4 (1C, s).

## (E)-3-(1-(benzo[d]oxazol-6-ylimino)ethyl)-8-methoxy-2H-chromen-2-one

Light green colour solid, M.P. 186 °C, yield 32 %. <sup>1</sup>H NMR: δ 2.37 (3H, s), 3.77 (3H, s), 7.15 (1H, dd, *J* = 8.0, 1.4 Hz), 7.35 (1H, dd, *J* = 8.0, 1.4 Hz), 7.43-7.58 (2H, 7.49 (dd, *J* = 5.8, 1.7 Hz), 7.52 (t, *J* = 8.0 Hz)), 7.79 (1H, dt, *J* = 1.7, 0.5 Hz), 8.01 (1H, dt, *J* = 5.8, 0.4 Hz), 8.20 (1H, t, *J* = 0.5 Hz), 8.35 (1H, s) <sup>13</sup>C NMR: δ 24.6 (1C, s), 55.8 (1C, s), 110.3 (1C, s), 113.8 (1C, s), 117.1 (1C, s), 120.4 (1C, s), 121.1 (1C, s), 123.7 (1C, s), 125.2 (1C, s), 130.9 (1C, s), 140.1 (1C, s), 142.9 (1C, s), 147.0 (1C, s), 147.3 (1C, s), 147.6 (1C, s), 152.6 (1C, s), 154.7 (1C, s), 159.1 (1C, s), 160.8 (1C, s)

## (E)-3-(1-((2,3-dihydrobenzo[b][1,4]dioxin-6-yl)imino)ethyl)-8-methoxy-2H-chromen-2-one

White colour solid, M.P. 176 °C, yield 22 %. <sup>1</sup>H NMR: δ 2.29 (3H, s), 3.81 (3H, s), 4.17 (2H, ddd, *J* = 13.7, 7.0, 1.8 Hz), 4.50 (2H, ddd, *J* = 17.8, 7.0, 1.8 Hz), 6.77-7.12 (4H, 6.83 (dd, *J* = 8.6, 0.5 Hz), 6.90 (dd, *J* = 8.6, 1.3 Hz), 6.94 (dd, *J* = 1.3, 0.5 Hz), 7.05 (dd, *J* = 8.2, 1.7 Hz)), 7.25 (1H, dd, *J* = 8.2, 8.1 Hz), 7.43 (1H, dd, *J* = 8.1, 1.7 Hz), 8.08 (1H, s). <sup>13</sup>C NMR: δ 24.6 (1C, s), 55.8 (1C, s), 64.2-64.3 (2C, 64.2 (s), 64.2 (s)), 98.2 (1C, s), 113.8 (1C, s), 117.3 (1C, s), 120.4 (1C, s), 123.7-123.8 (2C, 123.7 (s), 123.8 (s)), 125.2 (1C, s), 130.9 (1C, s), 132.6 (1C, s), 142.9 (1C, s), 143.3 (1C, s), 147.0 (1C, s), 147.3 (1C, s), 149.4 (1C, s), 159.1 (1C, s), 160.8 (1C, s)

## (E)-3-(1-(benzo[d]oxazol-2-ylimino)ethyl)-8-methoxy-2H-chromen-2-one

Light green colour powder, M.P. 180 °C. <sup>1</sup>H NMR: δ 2.31 (3H, s), 3.77 (3H, s), 7.15 (1H, dd, *J* = 7.7, 1.4 Hz), 7.31 (1H, dd, *J* = 8.0, 7.7 Hz), 7.44-7.67 (2H, 7.51 (ddd, *J* = 7.6, 7.5, 1.4 Hz), 7.60 (ddd, *J* = 7.9, 7.5, 1.7 Hz)), 7.75 (1H, ddd, *J* = 7.9, 1.4, 0.5 Hz), 7.85-8.08 (2H, 7.91 (dd, *J* = 8.0, 1.4 Hz), 8.02 (ddd, *J* = 7.6, 1.7, 0.5 Hz)), 8.65 (1H, s). <sup>13</sup>C NMR: δ 24.6 (1C, s), 55.8 (1C, s), 109.3 (1C, s), 113.8 (1C, s), 116.0 (1C, s), 120.4 (1C, s), 123.7 (1C, s), 124.4 (1C, s), 125.1 (1C, s), 125.2 (1C, s), 130.9 (1C, s), 142.9 (1C, s), 143.4 (1C, s), 147.0 (1C, s), 147.3 (1C, s), 149.2 (1C, s), 159.1 (1C, s), 160.8 (1C, s), 169.5 (1C, s).

## (E)-8-methoxy-3-(1-((1-methyl-6-phenyl-1H-benzo[d]imidazol-2-yl)imino)ethyl)-2H-chromen-2-one

Light green colour solid, M.P. 175-180 °C. <sup>1</sup>H NMR: δ 2.32 (3H, s), 3.82 (3H, s), 4.01 (3H, s), 7.13 (1H, dd, *J* = 7.6, 1.5 Hz), 7.43-7.71 (7H, 7.49 (tdd, *J* = 5.9, 1.9, 1.6 Hz), 7.51 (dd, *J* = 2.0, 0.4 Hz), 7.53 (dd, *J* = 7.9, 7.6 Hz), 7.62 (dddd, *J* = 7.1, 5.9, 1.9, 0.5 Hz), 7.64 (dddd, *J* = 7.1, 1.7, 1.2, 0.5 Hz)), 7.78-7.97 (3H, 7.83 (dd, *J* = 5.1, 0.4 Hz), 7.91 (dd, *J* = 7.9, 1.5 Hz), 7.92 (dd, *J* = 5.1, 2.0 Hz)), 8.37 (1H, s). <sup>13</sup>C NMR: δ 24.6 (1C, s), 32.9 (1C, s), 55.8 (1C, s), 113.8 (1C, s), 117.0-117.1 (2C, 117.1 (s), 117.1 (s)), 120.4 (1C, s), 123.7 (1C, s), 124.8 (1C, s), 125.2 (1C, s), 126.9 (2C, s), 128.2 (1C, s), 128.9 (2C, s), 130.9 (1C, s), 137.1 (1C, s), 137.3 (1C, s), 140.3 (1C, s), 142.5 (1C, s), 142.9 (1C, s), 147.0 (1C, s), 147.3 (1C, s), 159.1 (1C, s), 160.8 (1C, s), 164.4 (1C, s).

## (E)-3-(1-((1,6-dimethyl-1H-imidazo[4,5-b]pyridin-2-yl)imino)ethyl)-8-methoxy-2H-chromen-2-one

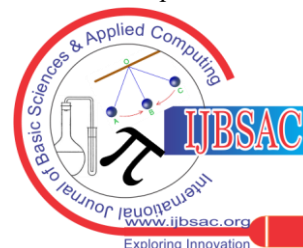
White colour powder, M.P. 195 °C. <sup>1</sup>H NMR: δ 2.15 (3H, s), 2.34 (3H, s), 3.77 (3H, s), 4.01 (3H, s), 7.15-7.37 (2H, 7.21 (dd, *J* = 7.6, 1.4 Hz), 7.30 (dd, *J* = 7.9, 7.6 Hz)), 7.91 (1H, dd, *J* = 7.9, 1.4 Hz), 8.08 (1H, d, *J* = 1.7 Hz), 8.52 (1H, s), 8.66 (1H, d, *J* = 1.7 Hz). <sup>13</sup>C NMR: δ 18.4 (1C, s), 24.6 (1C, s), 32.9 (1C, s), 55.8 (1C, s), 113.8 (1C, s), 119.5 (1C, s), 120.4 (1C, s), 123.7 (1C, s), 125.2 (1C, s), 130.4 (1C, s), 130.9 (1C, s), 139.9 (1C, s), 142.9 (1C, s), 144.6 (1C, s), 147.0 (1C, s), 147.3 (1C, s), 151.1 (1C, s), 159.1 (1C, s), 160.8 (1C, s), 164.4 (1C, s).

## IV. RESULTS AND DISCUSSION

### A. Analysis of Physicochemical Descriptors of Coumarin Schiff Base Derivatives 1-10

Several coumarin Schiff base derivatives have been designed as potential antimicrobial agents using a structure-based in silico approach. The physicochemical data of all compounds and standard antimicrobial agents (chloramphenicol, cycloheximide, nevirapine, and fluconazole) were calculated using the online Molinspiration and ChemDraw software. Some pharmaceutical-related properties and physicochemical descriptors, such as the number of hydrogen bond donors and acceptors, molecular weight, the octanol-water partition coefficient (log P), total polar surface area (TPSA), and the number of rotatable bonds, have been considered to evaluate the drug-likeness score of the compounds under study. Polar surface area (PSA) is a surface descriptor applied to measure the

permeability of drugs. The octanol-water partition coefficient (logP) is defined as a physicochemical parameter of hydrophobicity. Compounds with higher lipophilicity directly affect increased metabolism, as well as an increased possibility of toxicity. These factors are used to assess the acceptance of oral activity. All physicochemical or biological data of the Schiff base derivative were evaluated using Lipinski's rule of five. Lipinski's rule of five states that drug molecules should have a molecular weight ≤500, log p ≤5, hydrogen bond acceptor ≤10, hydrogen bond donor ≤5 and polar surface area ≤ 140 Å<sup>2</sup> [18]. The rule of five confirmed the bioavailability and the molecule designed in the library were assumed to have better intestinal permeability and good cell internalization. The entire designed compounds can ionise at a definite pH due to the presence of hydrogen bond donor and hydrogen bond acceptor sites, which are





C=N, C=O, and N-C dipoles that help increase the solubility of the compounds. The results (Tables 1 and 2) revealed that the compounds exhibited drug-like characteristics like those of standard antibiotics. Log P value, defining the lipophilicity of a compound, indicates the permeability of the drug through the cell membrane. The intermediate TPSA values of all compounds predicted good cell internalisation, similar to that of standard drugs. Molecules possessing more than one kind of violation are rejected because they are expected to have difficulty with bioavailability. The drug-

like properties for good bioactivity were also calculated for ion channel modulator, G-protein coupled receptor (GPCR), nuclear receptor ligand and kinase inhibitor (Table 2). Physicochemical results revealed that all the designed ligands adhered to the rule of five and were comparable to standard antibiotics, with some compounds even showing better results than the reference drugs. Therefore, all compounds were expected to exhibit lead-like properties, as shown in Table 2.

**Table I: Drug-Likeness Properties of Compounds 1-10**

Compounds	GPCR Ligand	Ion Channel Modulator	Kinase Inhibitor	Nuclear Receptor Ligand	Protease Inhibitor	Enzyme Inhibitor
1	-0.34	-0.16	-0.58	-0.45	-0.57	-0.13
2	-0.28	-0.09	-0.49	-0.21	-0.49	-0.00
3	-0.41	-0.22	-0.58	-0.40	-0.54	-0.18
4	-0.42	-0.20	-0.58	-0.40	-0.55	-0.20
5	-0.34	-0.22	-0.55	-0.40	-0.56	-0.17
6	-0.27	-0.24	-0.47	-0.18	-0.49	-0.06
7	-0.41	-0.17	-0.56	-0.37	-0.54	-0.23
8	-0.42	-0.30	-0.56	-0.38	-0.55	-0.25
9	-0.31	-0.18	-0.12	-0.67	-0.17	-0.32
10	-21	-.21	-0.32	-0.19	-0.21	-0.67

**Table II: Physicochemical Data of Compound 1-10**

Compounds	MW < 500	LogP ≤ 5	TPSA ≤ 140	HBA ≤ 10	HBD ≤ 5	Rotatable Bonds	Violation ≤ 1	Bioavailability Score
1	388.74	2.96	68.60	5	0	2	0	0.55
2	355.77	4.35	61.03	5	0	2	0	0.55
3	338.74	4.73	68.60	5	0	2	0	0.55
4	427.88	4.87	60.39	4	0	3	0	0.55
5	366.80	4.18	73.28	5	0	2	0	0.55
6	334.33	4.08	77.83	6	0	3	0	0.55
7	351.35	3.71	70.26	6	0	3	0	0.55
8	334.33	3.0	77.83	6	0	3	0	0.55
9	423.46	4.05	69.62	5	0	4	0	0.55
10	362.38	3.53	82.51	6	0	3	0	0.55
TPSA = total polar surface area, HBA = no. of H-bond acceptors, HBD = no. of H-bond donors, Violation = violation of Lipinski's rule of five.								

## B. In silico ADMET Prediction of Coumarin Schiff Base Derivatives 1-10

ADMET properties, including aqueous solubility (Log S), skin permeability (Log Kp), synthetic accessibility scores, and absorption (% ABS), were calculated using PkCSM software. In silico toxicity, pharmacokinetic and metabolic parameters of all coumarin Schiff base derivatives are predicted and summarized in **Table 3**. Intestinal absorption is greater than 75% for all compounds, surpassing the reference drugs cycloheximide (64.8%) and chloramphenicol (69.94%) [19]. Water solubility influences drug bioavailability, which is expressed as log S (mol/L). A compound that displays the value of water or aqueous solubility < (-) 4 is highly soluble [20]. Skin permeability is responsible for the transdermal delivery of drugs, which is represented by log Kp (cm/s or cm/h). A higher negative value of log Kp indicates a lower skin permeability of a drug or chemical compound [21]. The blood-brain barrier (BBB)

regulates the passage of chemical substances from the blood into the cerebrospinal fluid, which then enters the brain and spinal cord. The blood-brain barrier (BBB) process is measured as the log BB, which represents the logarithmic ratio of the brain-to-plasma concentration of the drug. The value log BB < (-) 1 indicated a poorly distributed drug in the brain. Metabolism plays a vital role in the bioavailability of drugs, and cytochrome CYP450 enzymes are the most crucial class to study this effect. Compounds were studied either to act as substrates or inhibitors of CYPs. Most of the designed compounds were found to be substrates for CYP3A4 and inhibitors of CYP1A2, CYP2C19, and CYP2C9. All ADMET parameters, including absorption, distribution, metabolism, excretion, and toxicity, revealed that all the designed ligands represented an acceptable range. In some cases, compounds showed even better results than reference drugs (**Tables 3 and 4**).

Table III: In Silico ADMET Predictions and Synthetic Accessibility of Compounds 1-10

Compound	Absorption		Distribution		Metabolism							Excretion		Toxicity	Synthetic Accessibility
	Water Solubility (log <sub>s</sub> mol/L)	Intestinal Absorption (Human) Numeric (%) Absorbed)	Skin Permeability Numeric (log Kp)	Blood-brain barrier Permeability (Log BB)	2D 6	3A4	1A2	2C19	2C9	2D6	3A4	Total clearance Numeric (log <sub>ml</sub> /mn /kg)	Renal OCT2 Substrate Categorical (Y/N)	Maximum tolerated dose (human) Numeric (Log <sub>mg</sub> /kg/day)	
					Substrate	Inhibitors				Categorical Y/N					
1	-5.00	97.18	-2.57	-0.60	N	Y	Y	Y	Y	N	Y	0.06	Y	-0.012	3.34
2	-5.18	97.75	-2.55	0.24	N	Y	Y	Y	Y	N	N	0.073	Y	-0.111	3.41
3	-5.58	95.57	-2.91	-0.29	N	Y	Y	Y	Y	N	N	-0.03	N	0.91	3.41
4	-2.90	87.45	-2.73	0.33	N	Y	Y	Y	Y	N	Y	0.43	Y	0.14	3.57
5	-2.96	96.31	-2.74	-1.02	N	N	Y	Y	Y	N	Y	0.46	Y	0.95	3.30
6	-5.07	97.23	-3.04	-0.45	Y	Y	Y	Y	Y	N	N	0.69	N	0.87	3.48
7	-5.09	98.71	-3.19	-0.37	N	Y	Y	Y	Y	N	N	0.47	N	0.76	3.69
8	-5.076	97.23	-3.04	-0.35	N	Y	Y	Y	Y	N	N	0.46	N	0.87	3.56
9	-3.75	97.72	-2.78	-0.63	N	Y	N	N	Y	N	Y	0.57	2.89	0.41	3.73
10	-2.74	98.93	-2.90	-0.87	N	Y	Y	N	Y	N	N	0.59	N	0.13	3.46
Water solubility = < -4 soluble; Intestinal absorption = Below 30 % indicates poor absorbance; Blood brain barrier permeability = < -1 considered poorly distributed to the brain; Skin permeability = > -2 considered to penetrate the CNS; Total Clearance (logCL <sub>tot</sub> ) = Lower value indicates high drug half lifetime; LD50 (Lethal Dose) = Lower value predicts minimum toxicity; Maximum tolerated dose = ≤ 0.47 predicts lower toxicity; Synthetic Accessibility = 1 (very easy) to 10 (very difficult)															

Table IV: Toxicity Predictions of Compounds 1-10 and Reference Drugs

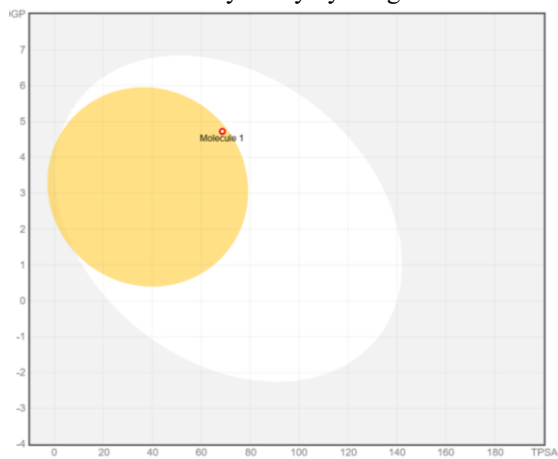
Compound	AMES Toxicity Categorical (Yes/No)	Max tolerated Dose(human) Numeric (log mg/kg/day)	hERG inhibitor Categorical (Yes/No)		Oral Rat Acute Toxicity LD50 Numeric (Mol/kg)	Oral Rat Chronic Toxicity (LOAEL) (Log mg/kg bw/day)	Hepatotoxicity Categorical (Yes/no)	Skin Sensation Categorical (Yes/no)	T.Pyriformis Toxicity Numeric (logug/L)	Minnow Toxicity Numeric (logmM)
			I	II						
1	Y	-0.12	N	N	2.05	2.05	Y	N	0.5	-2.26
2	Y	-0.111	N	N	2.45	2.45	Y-5	N		
3	N	0.91	N	Y	2.86	1.51	Y	N	1.07	0.34
4	Y	0.14	N	Y	2.48	0.07	N	N	0.28	-2.90
5	Y	0.95	N	Y	2.49	0.78	Y	N	0.28	-1.89
6	N	0.87	N	N	2.7	1.69	Y	N	0.93	0.60
7	N	0.76	N	Y	2.54	1.82	N	N	0.90	0.65
8	N	0.87	N	Y	2.7	1.69	Y	N	0.93	0.60
9	N	0.41	N	Y	2.89	2.12	Y	N	0.35	-0.47
10	N	0.13	N	Y	2.93	1.28	Y	N0	0.55	1.53

Ref.1= Donepezil Ref.2= Rivastigmine Ref.3= Tacrine LD50 = Lower value predicts minimum toxicity; Maximum tolerated dose = 0.47 predicts lower toxicity; AMES = Mutagenic or carcinogenic toxicity; LOAEL (Lowest adverse effect level test = LOAEL 10 mg per kg per day were labeled as substantial chronic toxicity, chemicals with LOAEL >50 mg per kg per day were labelled as weak chronic toxicity and chemicals with LOAEL ranged from 10 to 50 mg per kg per day were labeled as medium chronic toxicity. T. Pyriformis toxicity = Tetrahymena Pyriformis toxicity; Minnow toxicity = Acute fathead minnow toxicity is the basis of hazard and risk assessment for compounds in the aquatic environment. Structure-minnow toxicity relationship as follows:  $\log LC50 = 0.94 \log p + 0.94 \log (0.000068 p + 1) - 1.25$ , where p is the n-octanol/ water partition coefficient.

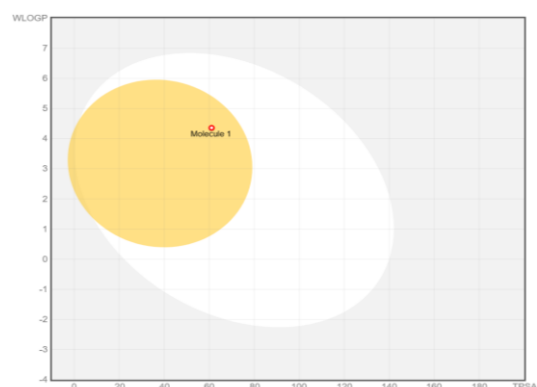
## V. BOILED-EGG MODEL

Brain access and gastrointestinal absorption are two essential pharmacokinetic behaviours that must be considered at different stages of the drug discovery process. For this purpose, the Brain or Intestinal Estimated permeation method (BOILED-Egg) is proposed as an accurate prediction model, which works by computing the polarity and lipophilicity of small molecules. The BOILED-Egg model, illustrated in Fig. 1, encompasses all compounds.

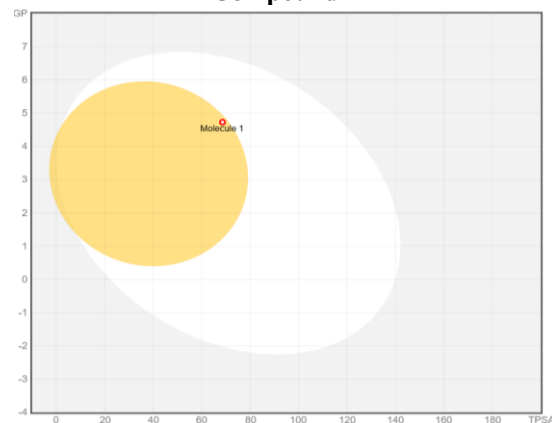
Compounds 1, 2, 3, 4, 5, 6, 7, 8, 9, and 10, which are present in the yellow zone, can permeate through the blood-brain barrier (BBB). All compounds present in the white area can be absorbed very easily by the gastrointestinal tract.



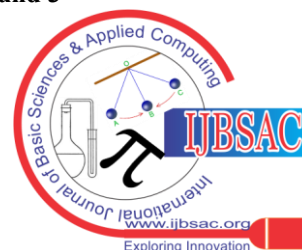
Compound 1

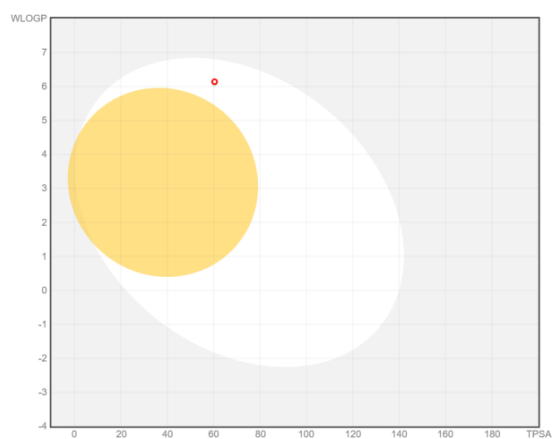


Compound 2

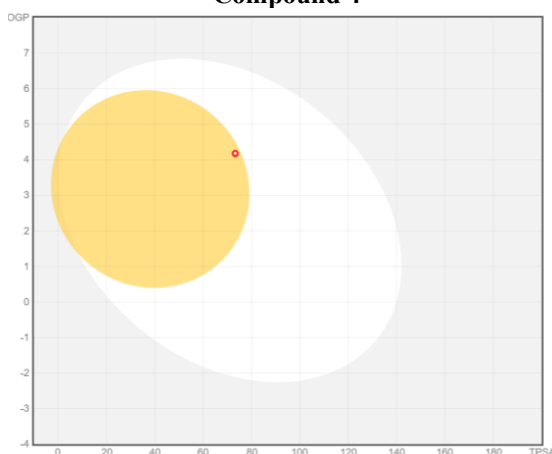


Compound 3

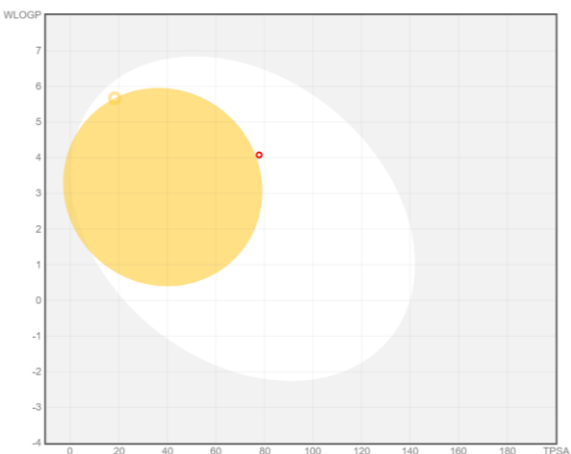




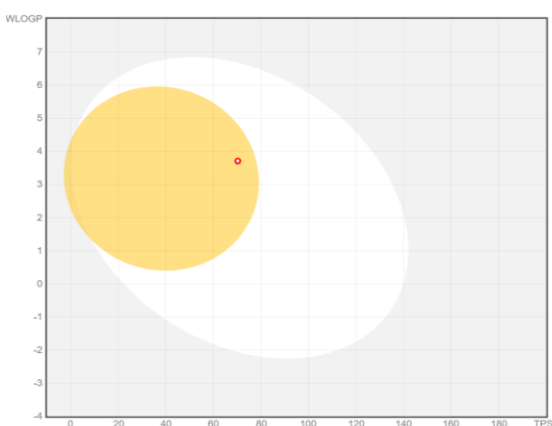
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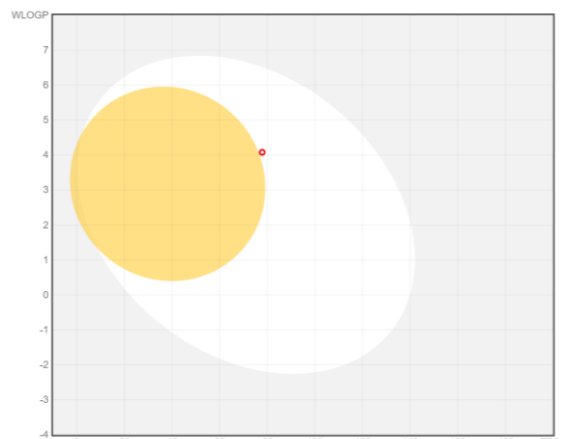
**Compound 5**



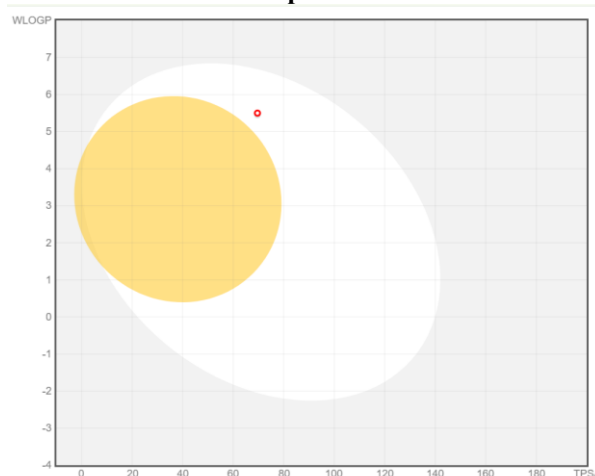
**Compound 6**



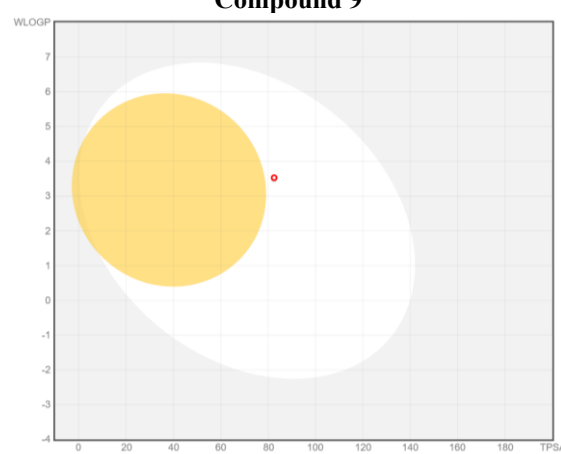
**Compound 7**



**Compound 8**



**Compound 9**



**Compound 10**

**[Fig.1: BOILED-Egg Model of the Coumarin Schiff Base Compounds 1-10]**

Compounds 1, 2, 3, 4, 5, 6, 7, 8, 9, and 10, which are present in the yellow zone, can permeate through the blood-brain barrier (BBB). All compounds present in the white area can be absorbed very easily by the gastrointestinal tract.

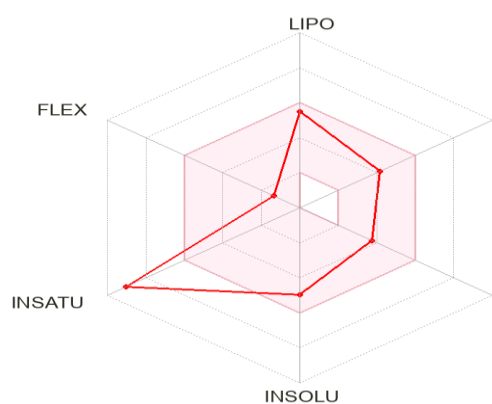
A transmembrane permeability glycoprotein (P-gp) is a member of the ATP-binding cassette (ABC) superfamily. P-gp functions as a carrier-mediated primary active efflux transporter. P-gp is distributed widely in the whole body and possesses a diverse range of substrates. Various therapeutic drugs are substrates to P-gp and them.

## Synthesis and Physicochemical Properties of Coumarin Derivatives as Antimicrobial Agents

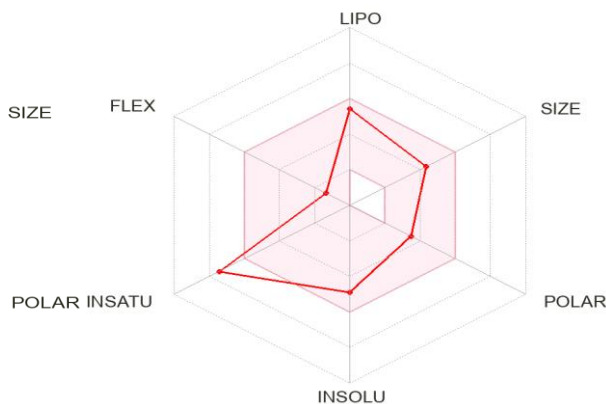
Bioavailability resistance is evoked due to protein efflux. Hence, P-gp inhibitors have been explored for overcoming the multidrug resistance and poor bioavailability problems associated with therapeutic P-gp substrates [22].

Physicochemical results (drug-like properties) of designed compounds may also be represented through radar graph using Swiss-ADME software (Fig. 2). Fig.2 Radar graph of isatin Schiff base derivatives 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, reference chloramphenicol and nevirapine (pink area reflect the permissible values for a drug molecule).

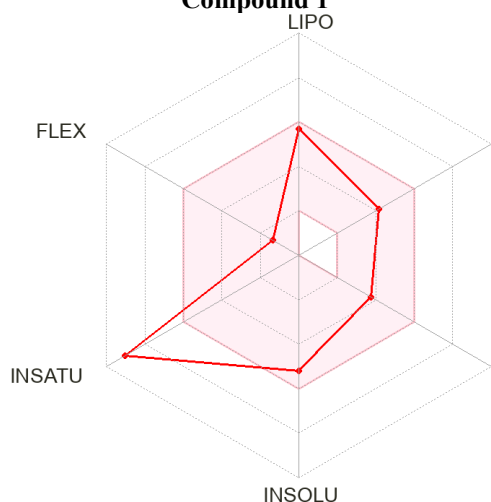
### VI. RADAR GRAPH



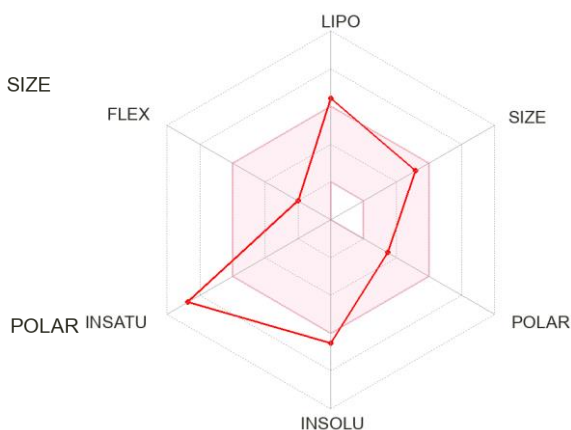
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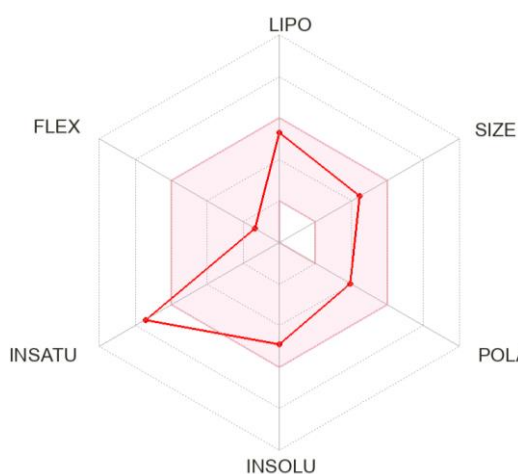
**Compound 2**



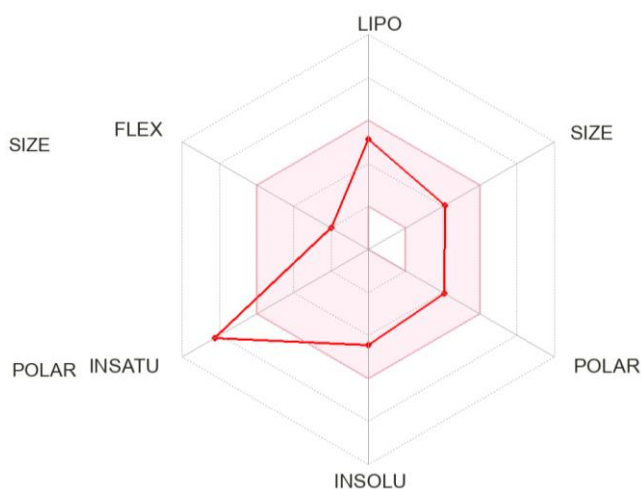
**Compound 3**



**Compound 4**

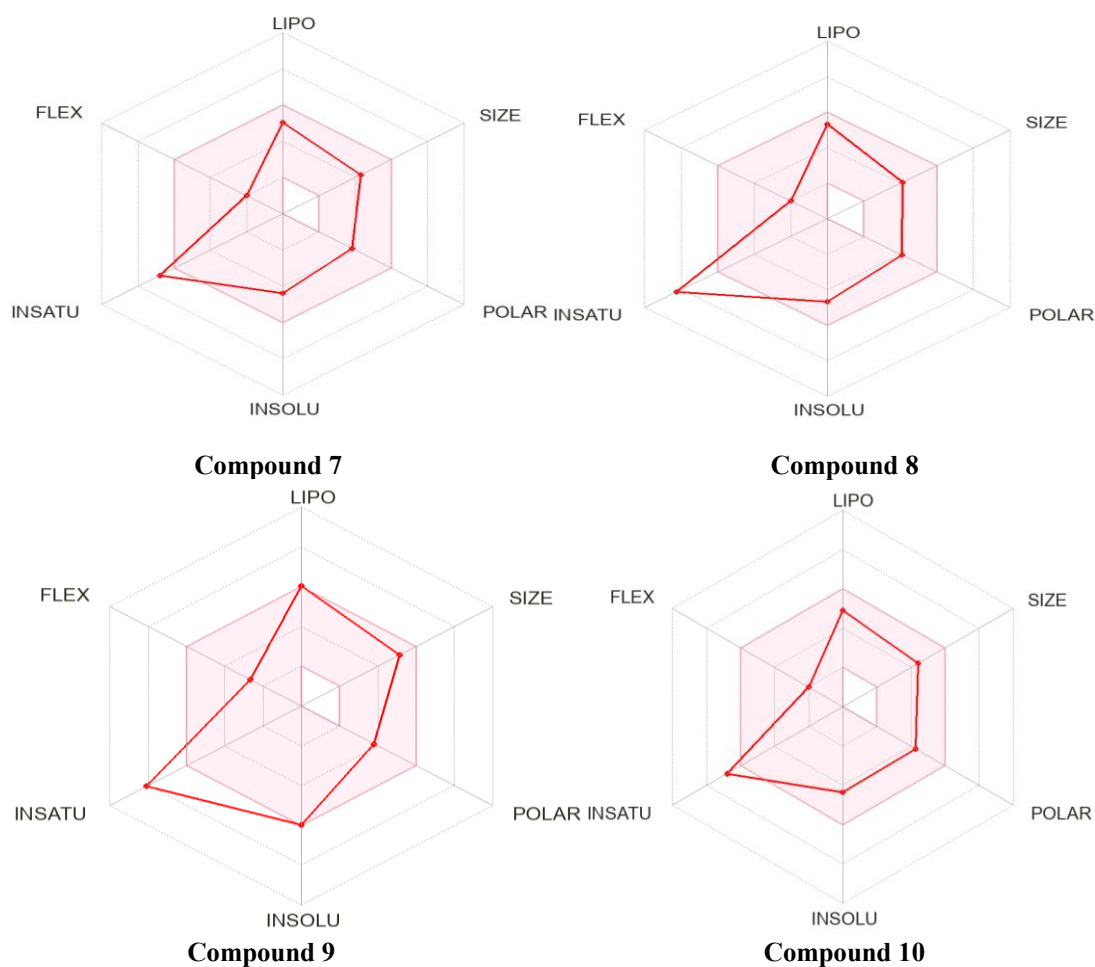


**Compound 5**



**Compound 6**

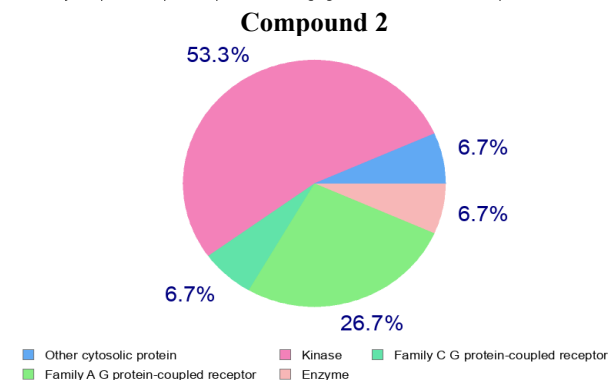
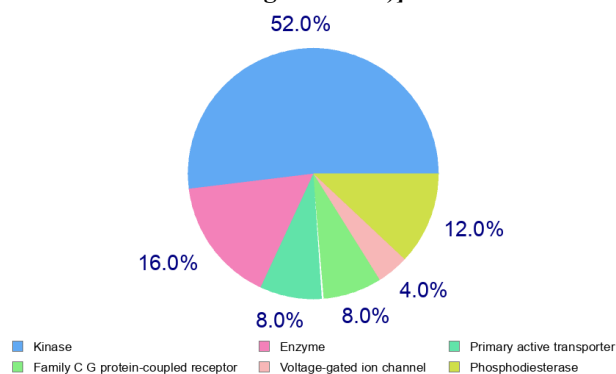
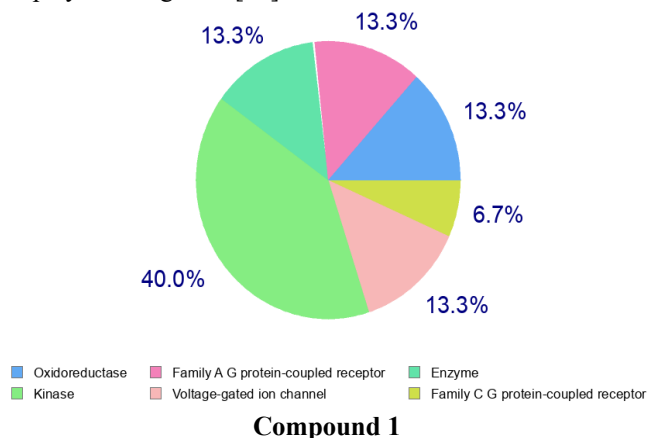




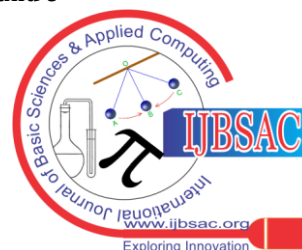
[Fig.2: Radar Graph of Coumarin Schiff base Derivatives 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, Reference Chloramphenicol and Nevirapine (Pink Area Reflects the Permissible Values for a Drug Molecule)]

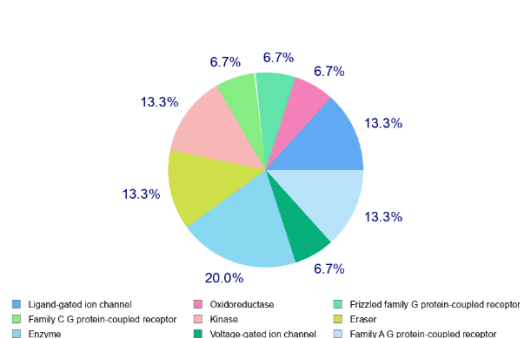
## VII. TARGET PREDICTION AND SWISS

The screening was done using Swiss Target Prediction against different targets such as kinase, protease, family A G protein-coupled receptor, secreted protein, phosphodiesterase, etc, for exploring future design (<http://www.swisstargetprediction>) (Fig. 3). We further used Swiss Similarity for in silico ligand-based virtual screening by using a combined method from ASINEX database (#693000) and ZINC (drug-like) method. Among all compounds, compounds 12 and 15 were found to be the most active; hence, the top three hits from each database are displayed in Figure 8 [23].

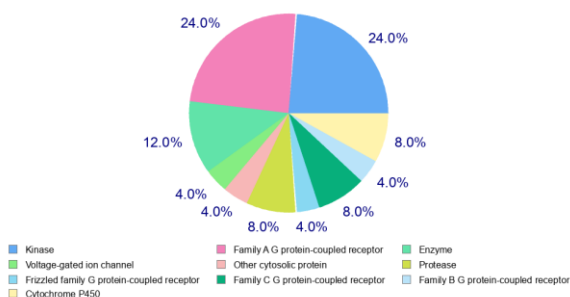


Compound 3

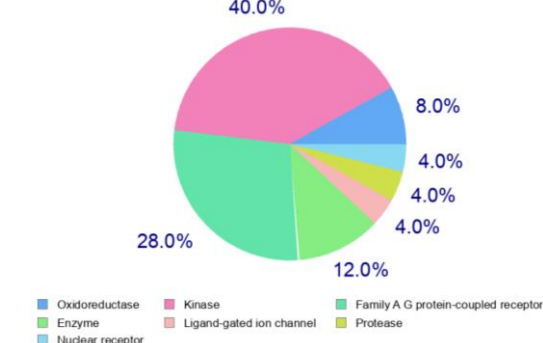




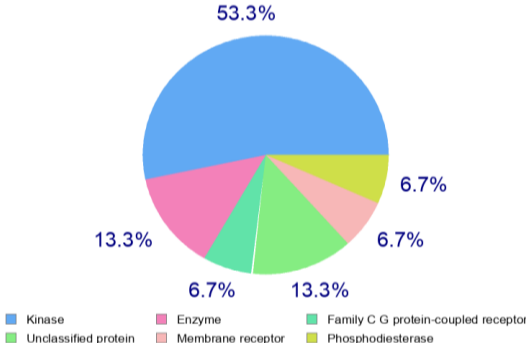
**Compound 4**



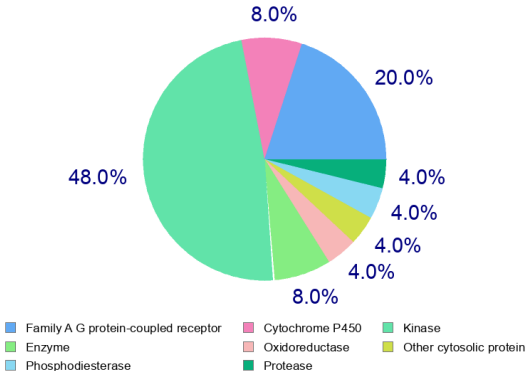
**Compound 5**



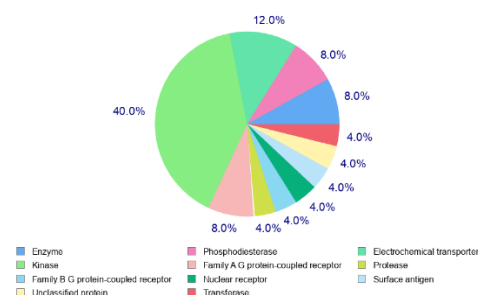
**Compound 6**



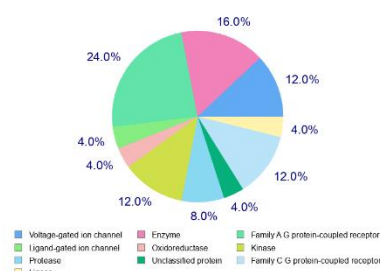
**Compound 7**



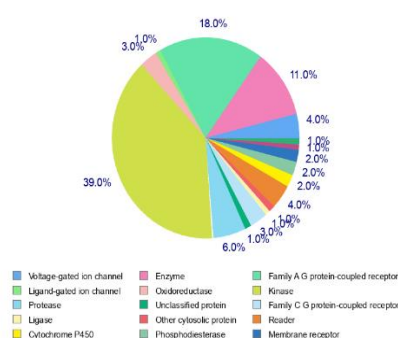
**Compound 8**



**Compound 9**



**Compound 10**



**[Fig.3: Swiss Target Prediction (Pie Chart) of a few Coumarin Schiff Base Compounds 1-10]**

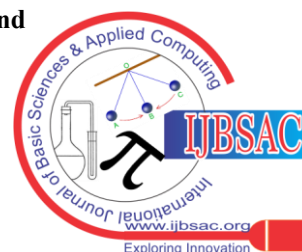
## VIII. CONCLUSION

Synthesized molecule exhibits promising antimicrobial activity, suggesting it as a valuable scaffold for further drug development. The combination of experimental data and computational insights suggests potential pharmacological benefits and supports further exploration of coumarine Schiff base compounds in medicinal chemistry.

## DECLARATION STATEMENT

After aggregating input from all authors, I must verify the accuracy of the following information as the article's author.

- **Conflicts of Interest/ Competing Interests:** Based on my understanding, this article has no conflicts of interest.
- **Funding Support:** This article has not been funded by any organizations or agencies. This independence ensures that the research is conducted with objectivity and without any external influence.
- **Ethical Approval and Consent to Participate:** The content of this article does not necessitate ethical approval or consent to participate with supporting documentation.
- **Data Access Statement and Material Availability:** The resources cited in this




article are publicly accessible.

- **Author's Contributions:** The authorship of this article is contributed equally to all participating individuals.

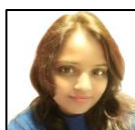
## REFERENCES

- article are publicly accessible.
- **Author's Contributions:** The authorship of this article is contributed equally to all participating individuals.
- ## REFERENCES
- Bazine I., Bendjedid S., Boukhari A (2020). Potential antibacterial and antifungal activities of novel sulfamido-phosphonate derivatives bearing the quinoline or quinolone moiety. In the Archiv Der Pharmazie. (Vol. 354, Issue-3) 2000291. DOI: <https://doi.org/10.1002/ardp.202000291>.
  - Shinde R.A., Adole V.A., Jagdale B.S., Pawar T.B. (2021). Superfast synthesis, antibacterial and antifungal studies of halo-aryl and heterocyclic tagged 2, 3-dihydro-1 H-inden- 1-one candidates. In the Monatshefte für Chemie-Chemical Monthly (Vol. 152, pp.649-658). DOI: <https://doi.org/10.1007/s00706-021-02772-0>
  - Faydy M. El, Dahaieh N., Ounine K., Lakhri B., Warad I., Tüzün B., Zarrouk A (2021). Synthesis, Identification, Antibacterial Activity, ADME/T and IBNA-Docking Investigations of 8-Quinolol Analogs Bearing a Benzimidazole Moiety. In the Arabian Journal for Science and Engineering (Vol. 47, Issue-10, pp. 1–14). DOI: <https://doi.org/10.1007/s13369-021-05749-7>.
  - Gajic I., Tomic N., Lukovic B., Jovicevic M., Kekic D., Petrovic M., Opavski N (2025). A comprehensive overview of antibacterial agents for combating Multidrug-Resistant bacteria: the current landscape, development, future opportunities, and challenges. In the Antibiotics (Vol.14, 221 Issue-3, pp. 1-40). DOI: <https://doi.org/10.3390/antibiotics14030221>.
  - Mishra R., Chaurasia H., Singh V.K., Naaz F., Singh R.K (2021). Molecular modelling, QSAR analysis and antimicrobial properties of Schiff base derivatives of Isatin. In the J. Mol. Str. (Vol. 1243, Issue-5, pp. 130763). DOI: <https://doi.org/10.1016/j.j.j.j.j.j.molstruc.2021.130763>.
  - Hetta H. F., Melhem T., Aljohani H. M., Salama A., Ahmed R., Elfadil H., Donadu M. G. (2025). Beyond Conventional Antifungals: Combating Resistance Through Novel Therapeutic Pathways. In the Pharmaceuticals (Vol 18, Issue 3, pp. 364). DOI: <https://doi.org/10.3390/ph18030364>
  - Manzoor S., Adnan T. R., Adnan Y. M., Cao W.-L., Tariq Q.-U.-N., Ali A., Ahmad N., Qiu C., Tian B., Zhang J.-G. (2023). Synthesis, Biological and Molecular Docking Studies of Pyrimidine-Derived Bioactive Schiff Bases. In the Bioorg. Chem., (Vol. 140) 106822. DOI: <https://doi.org/10.1016/j.bioorg.2023.106822>.
  - Toan V. N., Thanh N. D., Khuyen V. H. Tu L. T. C., Tri N. M., Huang N. T. T. (2021). N-(2,3,4,6-tetra-O-Acetyl-β-D-Glucopyranosyl) Thiosemicarbazones of 6-Alkoxy-2-Oxo-2H-Chromene-4-Carbaldehydes: Synthesis, Evaluation of Their Antibacterial, anti-MRSA, Antifungal Activity, and Docking Study. In the Med. Chem. Res. (Vol. 30, Issue-3, pp.1-17). DOI: <https://doi.org/10.1007/s00044-020-02688-0>.
  - Yang X.C., Zhang P.L., Kumar K. V., Li S., Geng R.-X., Zhou C.H. (2022). Discovery of Unique Thiazolidinone-Conjugated Coumarins as Novel Broad-Spectrum Antibacterial Agents. In the Eur. J. Med. Chem. (Vol 232,114192). DOI: <https://doi.org/10.1016/j.ejmech.2022.114192>.
  - Qin H.-L., Zhang Z.-W., Ravindar L., Rakesh K. P. (2020). Antibacterial Activities with the Structure-Activity Relationship of Coumarin Derivatives. In the Eur. J. Med. Chem.(Vol. 207, Issue-207, pp.112832). DOI: <https://doi.org/10.1016/j.ejmech.2020.112832>.
  - Basappa V. C., Penubolu S., Achutha D. K., Kariyappa A. K. (2021) Synthesis, Characterisation and Antioxidant Activity Studies of New Coumarin Tethered 1,3,4-Oxadiazole Analogues. In the J. Chem. Sci. (Vol. 133, Issue- 55). DOI: <https://doi.org/10.1007/s12039-021-01914-5>
  - Hamid, S. J., & Salih, T. (2022). Design, Synthesis, and Anti-Inflammatory Activity of Some Coumarin Schiff Base Derivatives: In Silico and In Vitro Study. In the Drug. Des. Devel. Ther. (Vol. 16, pp. 2275–2288). DOI: <https://doi.org/10.2147/DDDT.S364746>.
  - Song X.-F., Fan J., Liu L., Liu X.-F., Gao F. (2020). Coumarin Derivatives with Anticancer Activities: An Update. In the Arch. Pharm (Weinheim) (Vol. 353, Issue-8 e2000025). DOI: <https://doi.org/10.1002/ardp.202000025>.
  - Dai P., Wang Q., Teng P., Jiao J., Li Y., Xia Q., Zhang W. 2024. Design, Synthesis, Antifungal Activity, and 3D-QASR of Novel Oxime Ether-Containing Coumarin Derivatives as Potential Fungicides. In the J. Agri. Food Chem. (Vol. 72, Issue-11, pp. 5983–5992. DOI: <https://doi.org/10.1021/acs.jafc.3c06032>.
  - Naaz F., Srivastava R., Singh A., Singh V.K., Verma R., Singh R.K. (2018). Molecular modelling, synthesis, antibacterial and cytotoxicity evaluation of sulfonamide derivatives of benzimidazole, indazole, benzothiazole and thiazole. In the Bio. Med. Chem. (Vol. 26 Issue-12, pp. 3414–3428). DOI: <https://doi.org/10.1016/j.bj.2018.05.015>.
  - Srivastava R., Gupta S.K., Naaz F., Singh A., Singh V.K., Verma R., Singh R.K. (2018). Synthesis, antibacterial activity, synergistic effect, cytotoxicity, docking and molecular dynamics of benzimidazole analogues, Comp. In the Biol. Chem. (Vol. 76, pp.1–16). DOI: <https://doi.org/10.1016/j.compbiolchem.2018.05.021>.
  - Jacomini A.P., Silva M.J., Silva R.G., Gonçalves D.S., Volpato H., Basso E.A., Paula F.R., Nakamura C.V., Sarraggiotto M.H., Rosa F.A. (2016). Synthesis and evaluation against Leishmania amazonensis of novel pyrazolo [3, 4-d] pyridazinone-N-acylhydrazones-(bi) thiophene hybrids. In the European journal of medicinal chemistry (Vol. 124, Issue-, pp.340-349). DOI: <https://doi.org/10.1016/j.ejmech.2016.08.048>.Epub2016Aug23
  - Ghannay S., Kadri A., Aouadi, K. (2020). Synthesis, in vitro antimicrobial assessment, and computational investigation of pharmacokinetic and bioactivity properties of novel trifluoromethylated compounds using in silico ADME and toxicity prediction tools. In the Monatshefte für Chemie-Chemical Monthly (Vol. 151, Issue 2, pp. 267-280). DOI: <https://doi.org/10.1007/s00706-020-02550-4>
  - Klimoszek D., Jeleń M., Dołowy M., Morak-Młodawska B. (2024). Study of the lipophilicity and ADMET parameters of new anticancer diquinothiazines with pharmacophore substituents. In the Pharmaceuticals (Vol. 17, Issue 6, pp. 725- 745). DOI: <https://doi.org/10.3390/ph17060725>
  - Osborne, D. W., & Musakhanian, J. (2018). Skin penetration and permeation properties of Transcutol®—neat or diluted mixtures. In the AAPS PharmSciTech (Vol.19, Issue- 8, pp. 3512-3533. Epub2018Nov12. DOI: <https://doi.org/10.1208/s12249-018-1196-8>
  - Muhammed Aziz, D., & Ali Hassan, S. (2024). Synthesis, Characterisation, and Evaluation of Tetrazole Derivatives with Pyrrole-2, 5-Dione Moieties as Urease Inhibitors: Exploring Structure-Activity Relationships and Computational Insights. In the Chemistry Select (Vol. 9, Issue 23), e202401259. DOI: <https://doi.org/10.1002/slct.202401259>.
  - Sucularlı C., Tozkoparan B., Aytaç S. P. (2022). In silico activity and target prediction analyses of three triazolothiadiazine derivatives. In the Acta Medica (Vol. 53, Issue 3, pp.251-260). DOI: <https://doi.org/10.32552/2022.ActaMedica.737>
  - Zoete V., Daina A., Bovigny, C., Michielin, O. (2016). Swiss Similarity: a web tool for low to ultra high throughput ligand-based virtual screening. In the J Chem Inf Model (Vol. 56, Issue-8, pp. 1399-404). Epub 2016 Jul 19. DOI: <https://doi.org/10.1021/acs.jcim.6b00174>
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