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Synthesis, *Insilico* Study And Biological Evaluation Of Aurones And It's Analogue

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Abstract: Aurones are flavonoid compounds synthesized by plants as their secondary metabolite and potentially useful in many application such as antimicrobial, antioxidant, anti- inflammatory, anti- cancer ,antigout, etc. Aurones are synthesized from the formed chalcone which is then treated with mercuric acetate in presence of acetic acid by heating 110°. The formation of product is confirmed by TLC. Then carry out the anti-microbial study by disc plate method, gentamycin as standard, anti-oxidant study by hydrogen peroxide assay and anti-gout study by using xanthine extract from chicken liver and intestine. Docking of the synthesized compounds was performed by using PyRx software.

Index Terms - Aurones, Antimicrobial, Autodock by PyRx**.**

I. INTRODUCTION

Aurones are plant flavonoids that impart a yellow hue to the flowers of certain famous ornamental plants, including snapdragon and cosmos. Aurones are a category of natural substances present in plants, primarily within the Apiaceae family, which encompasses carrot, parsley, and celery. They are recognized for their vivid yellow hue and are frequently utilized in traditional medicine for their purported antioxidant and anti-inflammatory characteristics.

Aurones are flavonoid compounds characterized by their unique molecular structure, which includes a benzylidene moiety. They are synthesized by plants as secondary metabolites and serve various ecological functions, such as UV protection and defense against pathogens and herbbivores.

The process of creating a novel medication by molecularly altering a lead chemical to maximize the intended effect and reduce the adverse effects is known as drug design. Performed on computer or via computer simulation" is the term "*insilico*." The term "*insilico*" is a modern word usually experimentation performed by computer. It is described as the process of using a bioinformatics tool to identify the medication target molecule. Using the traditional procedure, an initial homology model is initially created in this approach.

II. EXPERIMENTAL WORK

Synthesis of Aurones:

Step 1: To prepare a chalcone, dissolve 2g of substituted ketone and 2.4g of substituted aldehyde has taken in a 10% sodium hydroxide solution. Stir the mixture in a magnetic stirrer for 4-6 hours until TLC indicates completion. The mixture is then poured into crushed ice, refrigerated, filtered, and dried. The compound is then recrystallized with ethanol and dried at room temperature.

Step 2: The compound then treated with mercuric acetate in acetic acid or pyridine at 110°C, poured into crushed ice. The solution kept in refrigerator for late night and filtered. Then dried at room temperature and recrystallized by using ethanol.

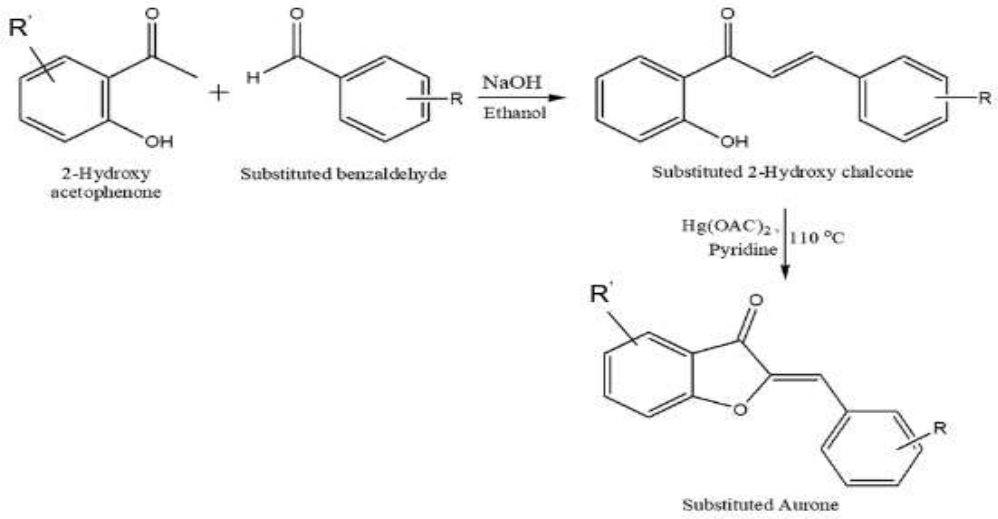

Figure 1: scheme for the synthesis of aurones

III. *INSILICO* STUDIES

The drug was designed and docked with the 3AX1 protein using PyRX 0.8 software, energy minimization of ligand was done by Chem 3D Pro it reveals a strong binding affinity between the designed molecules and the protein.

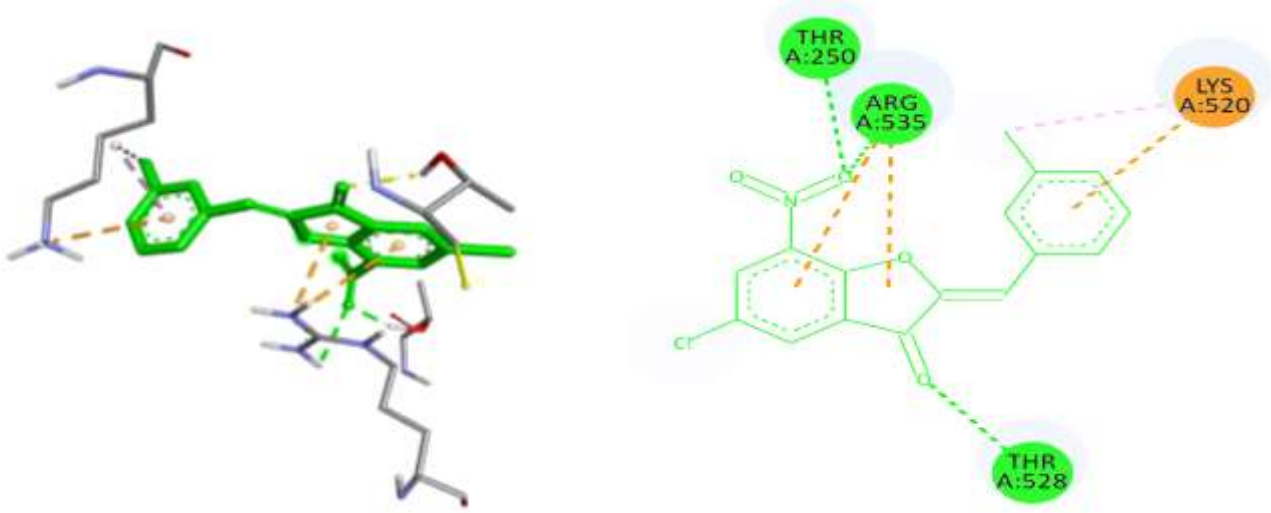

Figure 2: Docking Pose For Compound 1(C1)

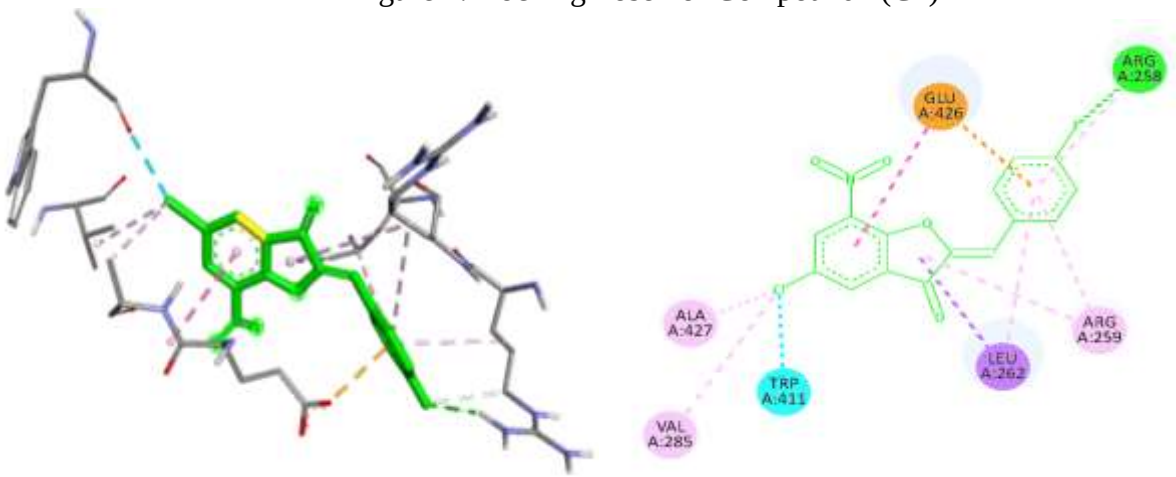

Figure 3: Docking Pose of Compound 2(C2)

The docking of designed molecules has been carried out and it shows the C1 has the lowest docking score of -8.9Kcal/mol while the C2 has a docking score of -8.1Kcal/mol. All the synthesized molecules show good binding energy with the protein xanthine oxidase reductase with a hydrogen bond interaction with the molecules.

Table 1: Docking score of synthesized compounds

Compound Code	Docking Score (Kcal/mol)
C1	-8.9
C2	-8.1
C3	-7.4
C4	-7.2

Antimicrobial study

Antibacterial activities of synthesized compounds were evaluated against *Bacillus Subitilis* (g+ve) and *Ecoli* (g-ve) and zone of inhibition was measured. Gentamycin was used as the standard drug for gram negative and ciprofloxacin as standard for gram negative bacteria. The compound C1 has shown a zone of inhibition of 2.5cm for gram positive and 2.0cm for gram negative bacteria. Other compounds have moderate activity when compared to the standards.

Table 2: Antimicrobial Study

Concentration of drug	Zone of inhibition	
	Bacillus Subitilis	*Ecoli*
Control	0	0
Standard	2.2	2.0
10	2	1.8
50	2.1	1.5
100	2.4	2
200	2.5	2.3

IV. ANTIOXIDANT ACTIVITY

The ability of the samples to scavenge hydrogen peroxide was determined according to the method of Ruch*i* et al (1989).Prepare the phosphate buffer by dissolving the appropriate amount of phosphate salts in distilled water to achieve *a PH of 7.4*. Dilute the compound to a suitable concentration usin*g* (100 µg/ml) phosphate buffer. Prepare a series of test tubes, each containing different concentration (10 µg/ml, 20 µg/ml, 30 µg/ml, 40 µg/ml and 50 µg/ml) of the compounds. Add a fixed volume (1ml) of hydrogen peroxide solution to each tube. Incubate the reaction mixture at room temperature for a specified period of time (10 minutes). Measure the absorbance of each compound at 520 nm using UV spectrophotometer.

Table 3: Absorbance of Antioxidant Activity by Hydrogen Peroxide

Concentration (µg/ml)	Absorbance (nm)
Blank	0
Standard (ascorbic acid)	0.089
10 µg/ml	0.292
20 µg/ml	0.536
30 µg/ml	0.777
40 µg/ml	1.027
50 µg/ml	1.281

CONCLUSION

The docking score of compound C1 against the xanthine oxidase protein is -8.9 Kcal/mol. The disc plate method was then used to measure the antibacterial activity. Gram positive bacteria have a zone of inhibition of 2.5 cm for compound C1, while gram negative bacteria have a zone of inhibition of 2.3 cm. The hydrogen peroxide assay was used to measure antioxidant activity, and it was observed that compound C1 had superior activity.

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