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"A Review on Aurone Derivatives as Potential Lead Compound for Drug Discovery"

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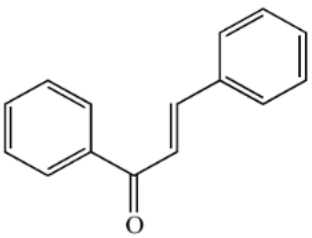
ABSTRACT: Aurone derivatives have gained significant attention in medicinal chemistry due to their wide range of biological activities and promising therapeutic potential. These compounds exhibit noteworthy anticancer, anti-inflammatory, antimicrobial, and neuroprotective properties, making them attractive candidates for drug development. This review provides a comprehensive overview of the current research progress on aurone derivatives as potential lead compounds in drug discovery. It summarizes the various synthetic approaches used for their preparation and highlights key structure–activity relationships governing their biological effects. Additionally, the pharmacological characteristics of aurone derivatives— including their absorption, distribution, metabolism, and excretion (ADME) profiles—are discussed. The review further explores their potential therapeutic applications in major disease areas such as cancer, neurodegenerative disorders, and infectious diseases. Despite their promising biological activities, several challenges remain in advancing aurone derivatives as lead molecules, particularly the need to optimize pharmacokinetic properties and reduce potential toxicity. Overall, this review outlines both the opportunities and limitations associated with the development of aurone-based therapeutics and offers perspectives for future research. Aurone derivatives represent a compelling class of molecules with substantial potential for the discovery and development of new therapeutic agents.

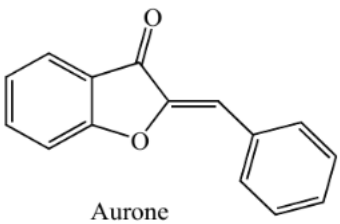
KEYWORDS: Aurone derivatives, drug discovery, medicinal chemistry, biological activities, therapeutic applications, structure-activity relationships, pharmacological properties.

I.INTRODUCTION

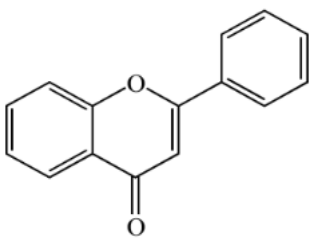
Aurones are a small but distinct class of flavonoids characterized by a benzofuranone core, typically formed through oxidative cyclization of chalcones. Although they occur less frequently in nature than other flavonoid subclasses, aurones contribute significantly to the yellow pigmentation of many flowers, serving ecological functions in pollinator attraction. In recent years, aurones have gained substantial scientific interest due to their broad spectrum of biological activities, including antioxidant, antimicrobial, anti-inflammatory, and anticancer effects. Their simple structural framework and tunable electronic properties also make them attractive for synthetic modification and structure–activity relationship studies. As a result, aurones have emerged as promising candidates for medicinal chemistry, photophysical research, and material science applications. The text appears to be discussing the synthesis of aurones, specifically two methodologies and the challenges associated with using heavy metal salts in the process. General structure of aurone



Chalcone



Aurone



Flavone

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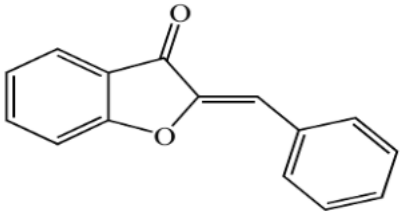
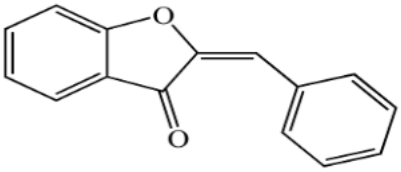
Isomer's of aurone

Aurones show only a few types of isomerism, mainly because of their rigid benzofuranone–benzylidene framework. The most important isomeric feature is the geometry around the exocyclic double bond. This double bond strongly favors the Z-configuration, which is also the form found in natural aurones. The E-isomer is theoretically possible but rarely observed because the planar system and intramolecular interactions stabilize the Z-form. Substitution patterns on both aromatic rings generate positional isomers, especially when hydroxyl, methoxy, halogen, or electron-withdrawing groups are introduced at different positions of the A- or B-ring. These positional changes can influence conjugation, electronic distribution, and biological activity.



Z-IsomerAurone



E-IsomerAurone

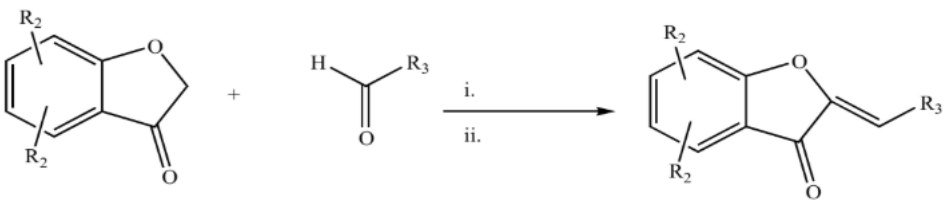
Some aurones can also show tautomeric behavior, although it is limited. The lactone ring can exist in equilibrium with an open-chain chalcone-like form under strong basic or acidic conditions, but under normal conditions the closed aurone structure is strongly favored. Structural analogues such as hemiacetal-like forms may appear transiently in solution, but they do not exist as stable, isolable isomers. Functional group substitutions, especially phenolic groups, can create intramolecular hydrogen bonds that further stabilize specific isomeric patterns and restrict the molecule to fewer conformational possibilities.

Aurones can be synthesized through two primary methods. The first involves condensing 3 coumarones with aldehydes, catalyzed by substances like alumina, alumina-potassium fluoride, barium oxide, or eutectic choline chloride-urea. The second method mirrors the biosynthesis of aurones, involving the oxidative rearrangement of chalcones with toxic metal salts such as thallium, mercury, or gold oxidants. However, heavy metal salts (Ba, Tl, Hg, Au) pose problems for drug preparation due to potential interference in biological tests. To address this, research has focused on green synthesis methods without heavy metals, extending work on 3-coumarone condensation. This aims to create novel aurones with groups like 2,3-dihydro-1,4-benzodioxin, 1,3-benzodioxol, and ferrocenyl, leveraging known biological properties of 2,3-dihydro-1,4 benzodioxine and 1,3-benzodioxole, though aurone derivatives of these remain unexplored.

1. Green synthesis of aurone

Karima baussafi and his coworker synthesized aurone by green synthesis

In this study, the goal was to prepare aurones using a greener method with minimal solvent. To achieve this, aurones were synthesized under solvent-free conditions using alumina or alumina–potassium fluoride as reaction support. Alumina–potassium fluoride acts as a stronger basic catalyst than alumina alone and usually gives better yields. But alumina was preferred when the substrate contained a free phenolic group. When potassium fluoride was used with coumaran-3ones that had a hydroxyl group, it formed a phenate potassium salt. That caused problems during aurone desorption, so plain alumina worked better in such cases. The solvent-free reactions moved faster under microwave heating, and the yields under microwave and classical heating were similar. All reactions showed stereospecificity. The compound obtained had the Z configuration, which matches the natural configuration of aurones.



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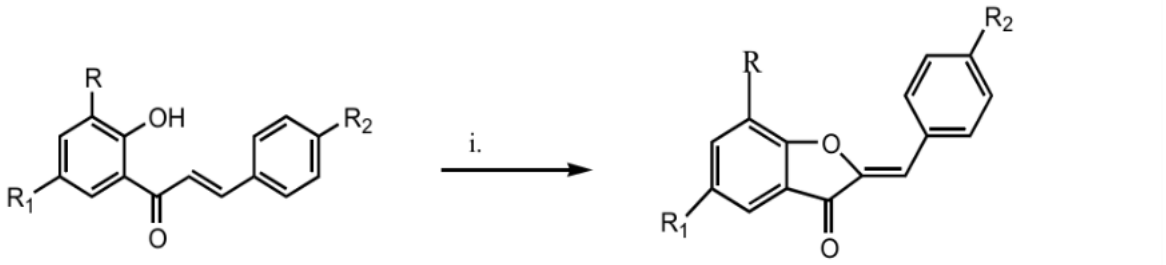
Scheme 1: reaction and condition i Al_2O_3-KF or Al_2O_3, ii Solvent free 50-70^{0}C or Microwave
$1R_1$= OH, R_2=H, $2R_1$ =OMe R_2=H, $3R_1$=OH, $4R_1$=OMe , R_2 =OMe 5 Naphthafuran –3(2H)-One a. Ferrocene Carboxaldehyde b. 1,3-benzaldehyde-5- Carboxaldehyde (piperonal) c. 1,4 benzodioxane-6-Carboxaldehyde d. 3,4,5, trimethoxybenzaldehyde.

2 From chalcones

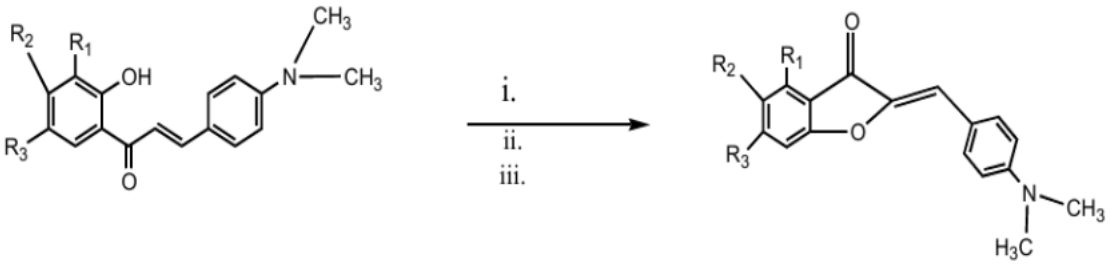
2.1. 1. $Hg(OAc)_2$

Agrawal etal. Described aurone were successfully obtained through oxidative cyclization of chalcones using ($Hg(OAC)_2$) mercuric acetate in pyridine, these aurone were further evaluated for their potential as anti-influenza agent as outlined in Scheme2.



Scheme 2 : Reagent and Condition cyclization of mercury (II) acetate in pyridine and cupric bromide in dimethyl sulfoxide

1	R	R_1	R_2
a	H	CH_3	H
b	Br	H	CH_3
c	Br	CH_3	OCH_3
d	H	CH_3	Cl



2.1. 2. Scheme 3 reaction condition : i) $Hg(OAC)_2$ ii) inDMSO iii) Reflux for 6 hr

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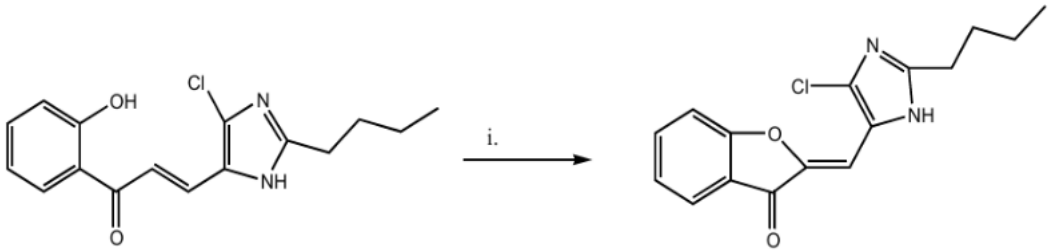
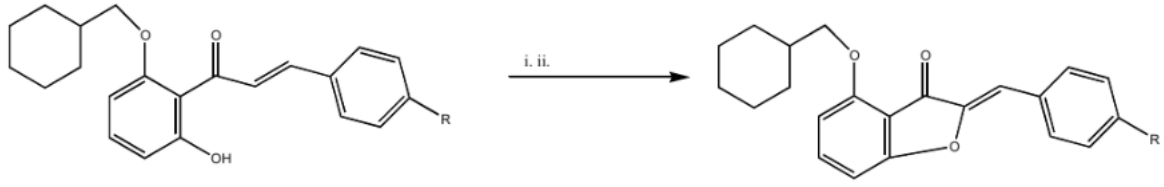
	R_1	R_2	R_3	Molecular formula
a	Cl	H	Cl	$C_{17}H_{13}Cl_2O_2N$
b	Cl	H	Cl	$C_{17}H_{13}IClO_2N$
c	Br	H	Cl	$C_{17}H_{13}BrClO_2N$
d	Br	H	Br	$C_{17}H_{13}Br_2O_2N$
e	H	H	Br	$C_{17}H_{14}BrO_2N$
f	H	H	Cl	$C_{17}H_{14}BrO_2N$
g	Br	CH_3	Cl	$C_{18}H_{15}BrClO_2N$
h	I	CH_3	Cl	$C_{17}H_{15}IClO_2N$
I	Cl	H	CH_3	$C_{17}H_{16}ClO_2N$
j	Cl	H	CH_3	$C_{17}H_{13}BrClO_2N$

2.1. 3. Synthesis of Aurone containing imidazole moiety by the oxidation of 2-Hydroxy Chalcones with mercuric II acetate in polyethylene glycol (PEG-400)



Scheme 4. Reagent and condition: i) Hg $(OAC)_2$ /PEG-400 Reflux 120-130^{0}C
Aurone containing imidazole moiety are synthesized by oxidizing 2-Hydroxy chalcone with mercuric (II) acetate in polyethylene glycol (PEG-400) at 120^0- 130^{0}C for 2 hours followed by by acidification and recrystallization from acetic acid to yield the pure product.

3. 1. Thallium nitrate (TTN)
synthesis of aurone from thallium nitrate



Scheme 5: reaction and condition: i) thallium (III) nitrate (TTN) methanol, overnight at rt; ii) hydrochloric acid 50^{0}C, 5H
R= -H, -CHO, -$COOCH_3$, -NO_2, -COOH
Thanigaimlai and Yong synthesized aurone by oxidizing 2 hydroxy 6-cyclohexylmethoxy chalcone with thallium nitrate in methanol followed by HCL and found that electron withdrawing group on ring B gave aurone while strong EDG produced isoflavone NMR confirmed the aurone structure oxidative cyclization method gave only two isomers.

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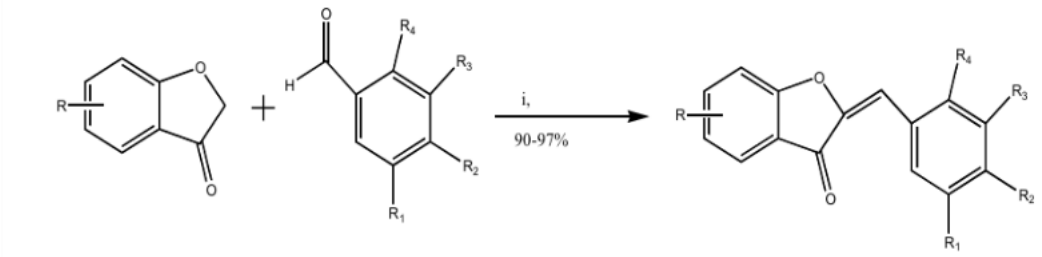
4. 1. From Resin

Synthesis of aurone from amberlite IR-120 Resin synthesized by Hoi Chen and coworker Amberlite catalyst catalyzed reactions are completed within 15-20 min in absence of amberlyst catalyst reaction time increased up to 48 hours no product formation takes place. Therefore, amberlite IR-120 resin catalyzed reaction was found to be advantageous in the present synthesis of aurone Benzofuran-3(2H)One and 4-6-dimethoxy-benzofuran-3(2H)-One Synthesized from corresponding phenols were the key starting material for this study. In presence of amberlite IR-120 resin in aqueous ethanol at 50^0C, aldol type condensation of compound with substituted benzaldehyde provides the corresponding product in excellent yields A series of 15 aurone derivatives were synthesized and evaluated for their anti-cancer activity against MDAMB-231 and MCF-7 cancer cell lines. Compound good anti-proliferative properties against the tested cancer cell line compared with standard among the synthesized compound.



Scheme: 6 Reagent and condition i) Amberlite IR-120 Resin 50% EtOH, 50^0C, 30Min

	R	R_1	R_2	R_3	R_4
a	H	H	H	H	H
b	H	H	H	NO_2	H
c	H	H	H	H	H
d	H	H	H	H	H
e	H	CH_3	CH_3	H	OH
f	H	H	OCH_3	H	OH
g	H	H	CH_3	H	H
h	H	H	Cl	H	H
i	H	H	H	OCH_3	H
j	H	H	H	H	OCH_3
k	H	H	H	OCH_3	OCH_3
l	H	H	F	H	H
m	H	H	CN	H	H
n	4,6- OCH_3	H	H	H	H
o	4,6- OCH_3	H	H	H	H

5. 1. preparation of 3-coumaranones 4 through fries rearrangement following synthesis of aurones

The most useful method of synthesis of aurones is condensation of 3-coumaranones with benzaldehydes Intermediate 3-coumaranones usually derive from phenols which can be easily converted into chloroacetic acid phenyl esters and further with varying success into ortho-hydroxy-α-halogen acetophenones in conditions of Fries rearrangement. Cyclization of intermediates proceeds readily in presence of bases resulting in 3-coumaranones. Reaction is synthesized by O.L. Kobzar et al.

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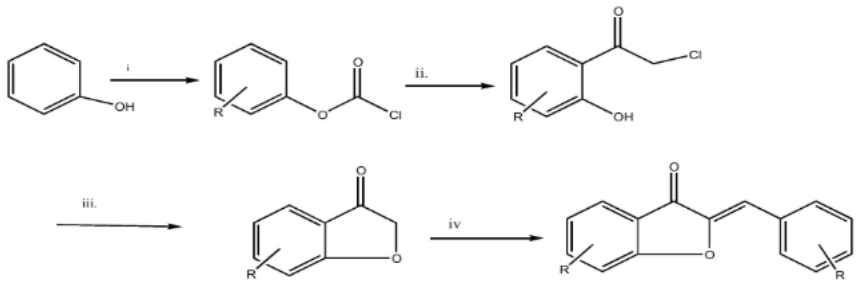


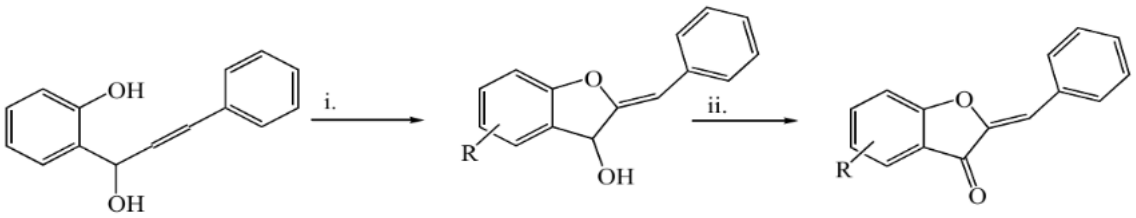
Scheme 7: reaction and condition i) $ClCH_2COCl$, 80-120^{0}C, 8h ii) AlCl 80-90^{0}C, 15Min iii) $AcoNa.3H_2O$ MeOH, 65^{0}C 1h, iv) RphCHO, ipr-OH, HCl. 80^{0}C, 2-8h

	R_4	R_5	R_6	R_7	$R_{2'}$	$R_{3'}$	$R_{4'}$
a	H	H	H	H	H	H	NO_2
b	H	H	H	H	H	NO_2	H
c	H	H	H	H	NO_2	H	H
d	H	H	H	H	H	OH	NO_2
e	H	H	H	H	H	NO_2	OH
f	H	H	H	H	OH	NO_2	H
g	H	H	H	H	OH	H	H
h	H	H	H	H	H	OH	OH
i	CH_3	Cl	CH_3	H	H	NO_2	OH
j	Cl	H	H	Cl	H	NO_2	OH
k	H	Cl	H	Cl	H	NO_2	OH

Aurone derivatives 5a–5k, functionalized with nitro groups, were evaluated in vitro as xanthine oxidase (XO) inhibitors. Introducing a hydroxyl group into the nitro-functionalized B-ring of these aurones resulted in a >20-fold increase in inhibitory potency toward the enzyme.

6. 1. Using Gold Catalyst

Harkat and Co-worker introduced derivative through alkylation, gold catalyzed cyclization and oxidation ,



Scheme 8 :reagent and conditions
i. Gold (I) catalyst MeCN , Rt
ii. Mno2, CH2Cl2, Rt , 1hr
A Gold (i) Catalyzed cyclization of 2 Cl Hydroxy-3 arypro-2ynyl, phenol was used to synthesis aurones, the process involved addition of lithium arylacitilyides to the phenols gold (i) mediated cyclization to an arylidene alcohol , and Mno2 oxidation to yield the aurone

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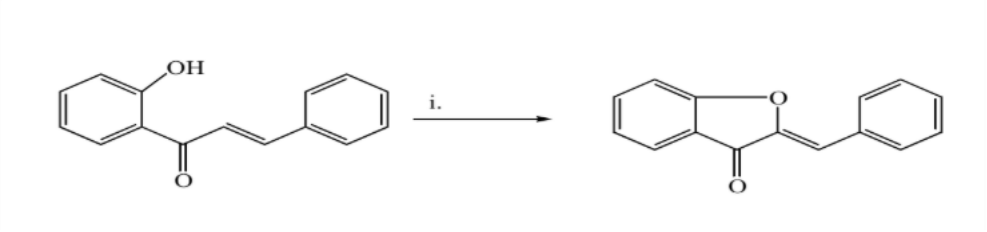
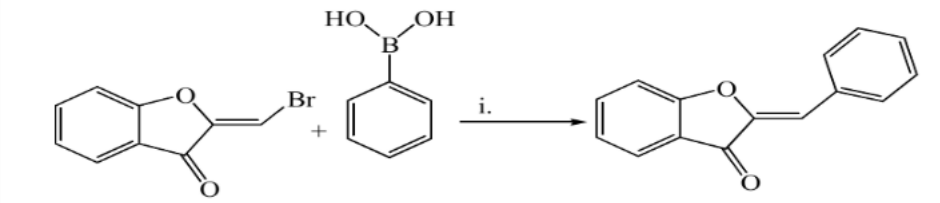
7. **1. From hydrogenperoxide**



Scheme 9; reaction and condition
i. H_2O_2 / OH, Methanol

This reaction is known as algar, flynn and oyamada (AFO) reaction . 2-hydroxychalcone oxidizes in the presence of alkaline hydrogen peroxide from epoxide as intermidiate which on attack yield aurones.

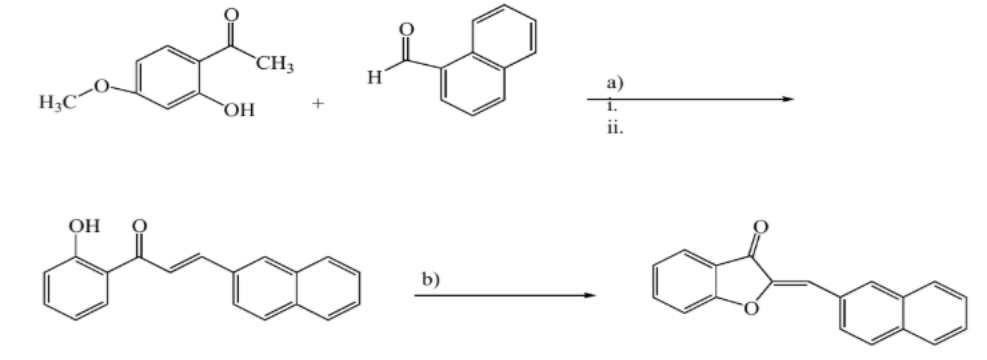
8. **1. Synthesis of aurone by suzuki cuppling**



Scheme 10 ; reagents and condition i) $Pd(PPh_3)_4$ (5 mol%), K_2CO_3, DMF Dioxane rt-90^{0}C
Suziki cuppling with phynel bromic acid provide aurone the suziki reaction is more commonly conducted with aryl iodide and bromide than with chloride

9. **1.Synthesis of AU-23 is a promising therapeutic option and a novel synthetic agent for treating bacterial infection and inflammation.**

Synthesized by Elsalami , et al .



Scheme 11: a) KOH 40 % W/V absolute EtOH i)Sonicate 1hr 40 ^{0}C ii) stir 25^{0}C 17hr
b) $Hg(OAc)_2$ DMSO 160 ^{0}C 6hr
Statastical data anylysis was performed using one way Anova followed by tukey's post hoc test all analysis were performed using graphical prism (version 9.0) the significance level was set at $p<0.005$.
The novel synthetic aurone AU-23 demonstrated promising antibacterial and anti-inflammatory properties showing bactericidal effect against sensitive bacterial stains (P aeruginosa and MSSA25923) and bactriostatic effects against MDR stains (MRSA43300 and MRSA33591). AU-23 also exhibits anti-inflammatory activity by reducing no

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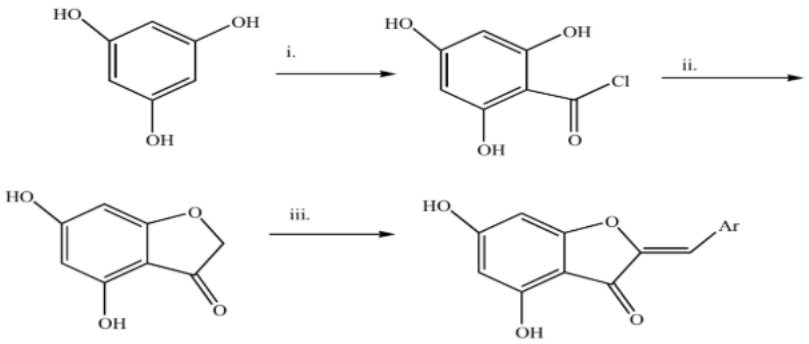
production, down regularity inflammatory makers (1L-6,1L-1B. INOS, TNF-a) vio the CD14 and TLR4 pathway the decresing intracellular POS content, making it a potential theraputic agent for treating bacterial infection and inflammation.

10. 1. **using Aldol condensation**

This reaction is synthesized by Marine peuchmaur et al.



Scheme 12: Genral pathway for the synthesis of aurone derivatives, reagent condition i) $ClCH_2CN$, HCl, $ZNCl_2$, Et_2o 0^0C ii) H_2O, 100^0C 5H ,84% (for 2 steps) iii) ArCHO, KOH 50% in H_2O, EtOH reflux 2-15H .

Aldol condensation takes place between arylaldehyde and 4,6-dihydrobenzofuran-3(2H)One under basic conditions. Reaction of phloroglucinol with chloroacetonitrile in HCl/Et_2O according to houben-housch reaction afforeded the chloroacetophenone which was directly cyclized in acidic media to afford the 4-6 dihydroxybenzofuron-3(2H)-One3 with 84% yeild for two steps.

BIOLOGICAL ACTIVITIES AND SAR TRENDS:

Aurones have emerged as versatile bioactive scaffolds, and recent studies highlight their wide-ranging biological activities along with clear structure–activity trends. In antimicrobial and antifungal research, a consistent observation is that hydroxyl substitutions tend to improve overall potency, especially by enhancing interactions with microbial enzymes. Electron-withdrawing groups have shown a marked increase in activity against Gram-positive bacteria, while halogenated aurones often display higher lipophilicity, enabling better membrane penetration. Because of these features, several aurone derivatives are being explored against resistant bacterial strains and difficult fungal pathogens. Their anticancer potential is equally significant. Many aurones exhibit cytotoxicity across multiple cancer cell lines and are known to trigger apoptosis through mitochondrial disruption or reactive oxygen species–driven pathways. Some structural variants also act as effective kinase modulators, which expands their relevance in targeted cancer therapy. Ongoing medicinal chemistry efforts focus on improving selectivity, lowering off-target toxicity, and enhancing metabolic stability.

Aurones also function as promising enzyme inhibitors. Their rigid, planar framework and ability to form hydrogen bonds allow them to fit well into active sites of enzymes such as tyrosinase, monoamine oxidase (MAO), kinases, and even certain viral proteases. These interactions open possibilities in treating pigmentation disorders, neurological diseases, and viral infections. In parallel, antiviral research has started drawing attention to aurones, with early studies reporting inhibition of viral enzymes and initial anti-SARS-CoV-2 activity. Structural analogues have shown broad antiviral potential, though more validation is needed before considering clinical applications.

From 2023 onward, a growing area of interest has been the neuroprotective and anti-inflammatory effects of aurones. Studies report reduced neuroinflammation, protection against oxidative stress in neuronal systems, and even improvements in cognitive markers in small-animal models. While these findings are still at an early stage, they suggest meaningful therapeutic promise. Overall, the evolving SAR trends and expanding biological profile make aurones a valuable platform for developing new antimicrobial, anticancer, antiviral, and neuroprotective agents.

CONCLUSION

Research on aurones and their derivatives demonstrates significant evolution in synthetic accessibility, photophysical exploitation, and biological application. The combination of rigid aromatic framework, tunable electronic features, and

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straightforward derivatization makes aurones an attractive platform for chemical biology, drug discovery, materials science, and photochemistry. While challenges remain— particularly pharmacokinetic liabilities—ongoing innovation positions aurones as a versatile and rapidly expanding chemical class.

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