ORIENTAL JOURNAL OF CHEMISTRY
An International Open Access, Peer Reviewed Research Journal
www.orientjchem.org
ISSN: 0970-020 X
CODEN: OJCHEG
2025, Vol. 41, No.(4):
Pg. 1305-1309

Synthesis and Biological Study of S-triazines from Chalcones

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http://dx.doi.org/10.13005/ojc/410427

(Received: May 01, 2025; Accepted: July 19, 2025)

ABSTRACT

A series of novel S-triazine derivatives were synthesized through a multi-step reaction. The process began with the reaction of cyanuric chloride and p-methoxyphenol, followed by interaction with 1-(5-hydroxyphenyl) ethenone and various aldehydes to form chalcone intermediates. These chalcones were then reacted with 2-aminobenzimidazole to yield the desired S-triazine derivatives. Characterization of all prepared compounds are done using spectroscopic method which includes proton NMR, carbon-13 NMR, Infrared and Mass spectroscopy. All prepared compounds were screened for their antibacterial activity against gram positive and gram negative bacteria.

Keywords: Antimicrobial activity, Cyanuric chloride, 2-Aminobenzimidazole; S-triazine.

INTRODUCTION

Heterocyclic compounds, a complex and diverse area within organic chemistry, are classified into two main categories: alicyclic and aromatic. These compounds have seen remarkable advancements in their study due to their widespread presence in nature, distinct chemical reactivity, and significant applications in medicine. They serve as valuable building blocks for incorporating biologically active groups. The intriguing biological activities of heterocycles have sparked considerable research, particularly in the context of their synthetic potential. Many natural substances derived from plants and animals, including alkaloids (nitrogen-containing bases) and glycosides, contain heterocyclic structures. These compounds have been utilized for medicinal purposes for centuries.

Pyrimidines, in particular, exhibit a range of therapeutic properties, such as anticancer[1-3], anti-inflammatory[4], anticancer, antihypertensive, antimicrobial[6-8], and antifungal effects. Studies suggest that various substituents at the 2/3 positions of the quinazolinone nucleus can significantly influence their pharmacological activity. Although several synthetic methods have been developed for preparing substituted pyrimidines, many of these approaches face challenges such as low yields, harsh reaction conditions, long reaction times, and difficulties in isolating the final products.

Present papers represent synthesis of novel s-triazine derivatives obtained from chalcones and 2-aminobenzimidazole. All synthesized compounds were characterized using various spectroscopic techniques. Present work also cover biological study

of synthesized compounds in terms of antimicrobial activity against gram positive and negative bacteria.

MATHODS AND MATERIALS

Reagents & Chemicals

Chemicals utilized in the experiments were of analytical grade and were used without additional purification. The reagents included various aldehydes, cyanuric chloride, 1-(5-hydroxyphenyl)ethenone, ethanol, p-methoxyphenol, 2-aminobenzimidazole, and sodium hydroxide, all sourced from Merck, Mumbai, India. All solvents were also obtained from Merck, Mumbai, India, and used as received.

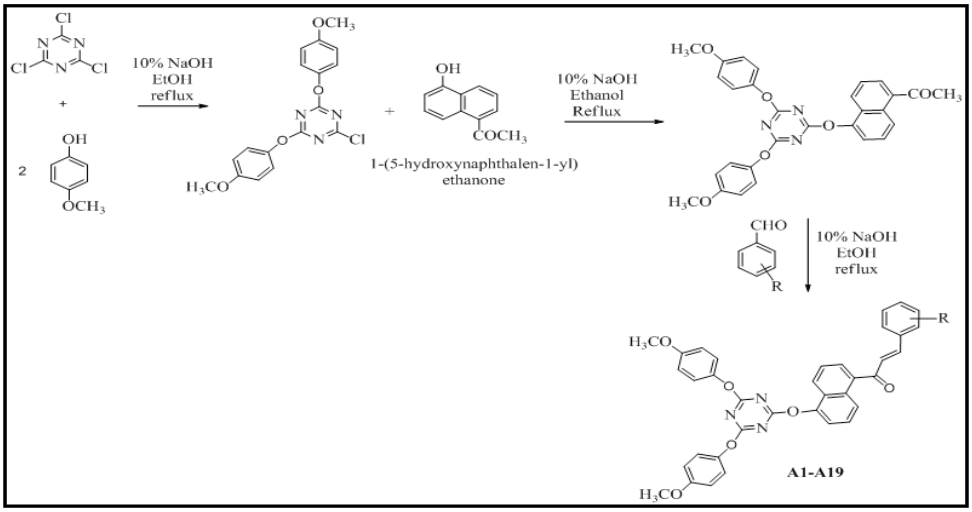
Experimental

For ^{1}H NMR analysis, a Bruker Avance-400 spectrometer was employed, while the carbon-13 NMR spectra are recorded with instrument having frequency 100 MHz and chemical shift are reported in parts per million unit. The infrared (IR) spectra were obtained using an FT-IR 3000 spectrophotometer from ABB Bomem Inc., with the results expressed in cm^{-1}. Mass spectrometry was performed using a Shimadzu LCMS-2010 system.

Synthesis Procedure

Synthesis of chalcones A1-A19

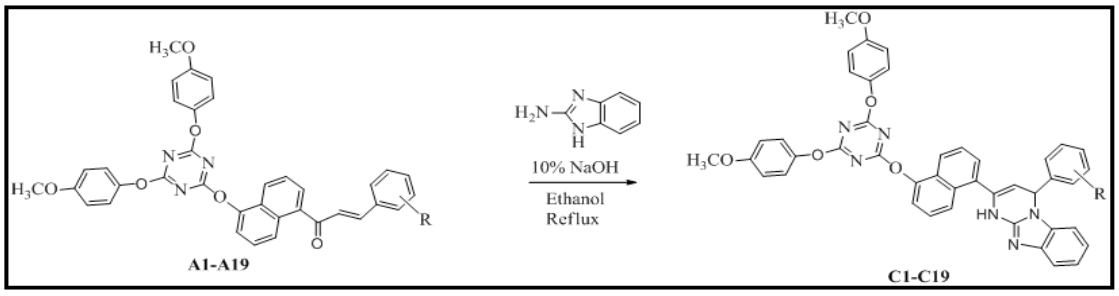
0.1 mole Cyanuric chloride and 0.2 mol methoxy phenol are dissolved in 75 mL sodium hydroxide at temperature 25°C with constant stirring. After dissolution is completed, the entire content were refluxed for 2 h under ethanol as the solvent and then add 0.01 mol 2-chloro-4,6-bis (4-methoxyphenoxy)-1,3,5-triazine (0.01 mol) and various aldehydes to obtained various chalcones A-1 to A-19 (Scheme 1).



Scheme 1. Symthesis of Chalcones A1-A19

Synthesis of C1-C19 (s-triazines)

0.01 mol chalcones were taken in 40 mL methanol and add 10% 40 mL sodium hydroxide with constant stirring followed by addition of 0.01 mol2-aminobenzimidazole and further refluxed for 1-2 h using ethanol as the solvent. Cooled the entire solution under ice cold water and crystalized product using ethanol as the solvent. TLC is used to checked reaction completion. Obtained product called C-1 to C-19 (Scheme 2).



Scheme 2. Synthesis of Striazines C1-C19

Table 1: Synthesis of s-triazines C-1 to C-19

Sr. No	s-triazines	R	Reaction Time (h)[a]	% Yield[b]	m. p. (°C)
1	C-1	-H	2	77	256
2	C-2	-4-OH	2	75	262
3	C-3	-3-OH	2	72	251
4	C-4	-2-OH	2	76	254
5	C-5	-2-OCH_3	2.5	80	242
6	C-6	-4-OCH_3	2.5	74	243
7	C-7	-2-Cl	2	84	245
8	C-8	-4-Cl	2	82	260
9	C-9	-3-Cl	2	80	255
10	C-10	-2-NO_2	1.5	85	230
11	C-11	-4-NO_2	1.5	86	220
12	C-12	-3-NO_2	1.5	84	218
13	C-13	-3-Br	2	84	252
14	C-14	-2-Br	2	80	245
15	C-15	-4-Br	2	82	230
16	C-16	-3, 4-$(OCH_3)_2$	2.5	75	228
17	C-17	-3,4,5-$(OCH_3)_3$	2.5	73	232
18	C-18	2-furfuryl[c]	2	84	244
19	C-19	2-Thineyl[c]	2	80	228

[a]Reaction is monitored by TLC, [b]Isolated yield & [c]Names of aldehyde groups

RESULTS AND DISCUSSION

Table 1 presents the different condensation products formed through the reaction between chalcones and 2-aminobenzimidazole. The data indicate that compounds containing electron-withdrawing groups undergo synthesis more rapidly than those with electron-donating groups. Specifically, compounds C10–C12, which possess electron-withdrawing substituent's, were synthesized approximately 1.5 h faster than compounds C16 and C17, which contain electron-donating groups and required about 2.5 hours. Notably, the highest yields were obtained from aldehyde derivatives with strong electron-withdrawing groups, such as nitro-substituted compounds.

Antimicrobial activity

Media Preparation

Nutrient agar was employed to assess biological characteristics of prepared compounds. The medium was prepared using the following composition:

- Agar-Agar: 15 g
- 5 g Peptone
- 3 g Metal extract
- 5 g Sodium hydroxide
- Distilled Water: 1000 mL

To prepare the medium, peptone was initially dissolved in distilled water, followed by the addition of the remaining components. The mixture was brought to a boil to ensure complete dissolution. Sterilization was performed using an autoclave at 125°C under 15 psi pressure for 20 minutes. Once cooled to approximately 45°C, under the pH 7-7.5, Add 20 mL sterilized medium in petri dish.

For microbial culture preparation, a nutrient broth was used, consisting of:

1. 10 g peptone
2. 10 g Beef Extract
3. 5 g NaCl

These components were dissolved in distilled water to support bacterial growth in the antimicrobial testing process.

Data of Antibacterial Study

Table 2: Date of Antibacterial study of Compounds C-1 to C-19

Compounds	Gram+ve *S. aureus*	Gram+ve *B. megaterium*	Gram-ve *E. coli*	Gram-ve *P. vulgaris*
C1	8	3	4	5
C2	9	9	11	8
C3	12	13	14	12
C4	9	8	8	6
C5	7	7	8	8
C6	8	9	7	6
C7	9	14	12	9
C8	11	12	9	10
C9	12	13	10	13
C10	14	6	5	7
C11	7	10	7	7
C12	8	8	8	8
C13	9	7	3	11
C14	4	6	11	4
C15	10	7	8	8
C16	8	4	7	6
C17	7	6	10	12
C18	9	10	12	3
C19	12	11	4	8
Ampicillin	15	14	17	19
Gentamycin	16	15	14	16

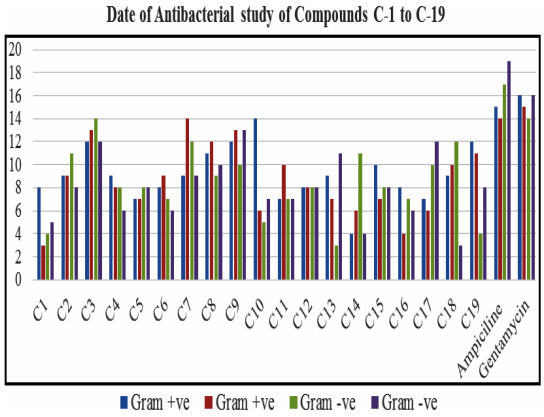
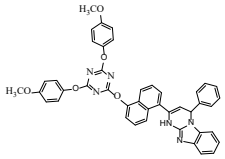


Fig. 1. Antimicrobial study of compound C-1 to C-19

Characterization

Compound: C1	
Molecular formula: $C_{43}H_{32}N_6O_5$	
m. p. (°C):	256
^{1}H NMR (400 MHz, $CDCl_3$) δ ppm	2.2 (1H, d, CH proton), 3.5 (6H, s, $-OCH_3$), 4.9 (1H, s, vinylic), 6.2-8.4 (23H, Ar-H, m), 9.1 (NH, s).
13C NMR (100 MHz, $CDCl_3$) δ ppm	40.42, 52.6, 60.2, 63.4, 127.5, 128.1, 129.3, 130.1, 131.4, 136.9, 138.5, 139.2, 142.7, 143.4, 144.6, 151.8, 152.4, 152.8.
IR cm^{-1} (KBr)	3350, 3082, 2972, 1642, 1620, 1615, 1613, 1590, 1569, 1214, 740
Mass (m+1)	712.1
Elemental analysis	Calculated(%): C:72.46; H: 4.53; N:11.79 Found(%): C: 72.75; H: 4.91; N: 11.95

Compound C1 was selected as the representative molecule for spectral analysis. Proton NMR spectroscopy shows signals for each proton and proton possess group. were identified, based on the principles of shielding and deshielding. Aromatic protons of the compound appeared in the downfield region, with chemical shift values ranging between 6 to 8 ppm, while the proton associated with the $-OCH_3$ group was observed at approximately 3.5 ppm. Detailed ^{1}H NMR, ^{13}C NMR, IR, and MASS spectrometric data for compound C1 are provided above.

CONCLUSION

A series of highly functionalized s-triazine derivatives (C1–C19) were successfully synthesized through the reaction between 2-aminobenzimidazole and chalcones. Chalcones are prepared using different aromatic aldehyde. All the prepared compounds are confirm using characterization by various spectroscopic methods and tested them for biological activity. Based on the findings, these compounds show potential as lead candidates for anti-inflammatory drug development and warrant further investigation, including detailed toxicological assessments in future studies.

ACKNOWLEDGEMENT

I am glad to my research supervisor Dr. Gurang Jani sir for their valuable guidance and support. I also acknowledge, Principal, Arts, Science & Commerce College, Pilvai for providing necessary infrastructure for the research work. I also thankful to HOD, Department of Chemistry, Hemchandracharya North Gujarat University, Patan for all necessary support.

Conflict of interest

It is declared that, Author does not have any conflict of interest.

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