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Study of Synthesis and Antimicrobial Activity of Cynuricchloride Based 1,2,4-Triazoles

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ABSTRACT

The study of heterocyclic systems is of great interest both from the theoretical and practical point of view. Heterocyclic chemistry is an integral part of the chemical sciences and constitutes a considerable part of the modern researches. Triazole is 5-membered heterocycle containing three nitrogen atoms present at 1,2 and 4th position of the ring. It can be viewed as a derivative of cyanuricchloride based heterocycles. Compounds containing this functional group are useful commercially in analgesics and dyes. In the presence study we have synthesized various 1,2,4-triazoles from novel chalcones upon condensation reaction with 4H-1,2,4-trizoles-3-amine in the presence of NaOH as the base under ethanol solvent. All synthesized compounds were tested for their antimicrobial activity against gram positive and gram-negative bacteria. All the synthesized compounds were characterized by ^{1}HNMR, ^{13}CNMR, IR, MASS spectroscopic techniques.

Keywords: 1,2,4-Triazole, Chalcone, Antimicrobial Activity, Aldehydes and Cyanuric Chloride.

INTRODUCTION

Triazoles are a significant class of five-membered heterocyclic compounds containing three nitrogen atoms and two carbon atoms within the ring. Depending on the position of the nitrogen atoms, triazoles exist in two regioisomeric forms: 1,2,3-triazoles and 1,2,4-triazoles. These isomers exhibit distinct chemical and biological properties, making them valuable in diverse fields such as medicinal chemistry, agriculture, and materials science **[1, 2]**.

The synthetic versatility and chemical stability of triazoles have garnered substantial attention in organic and medicinal chemistry. Among the most prominent synthetic methods is the Huisgen 1,3-dipolar cycloaddition between azides and alkynes, particularly in its copper(I)-catalyzed variant (CuAAC), which provides regioselective access to 1,4-disubstituted 1,2,3-triazoles under mild conditions **[3, 4]**. This reaction, popularized by Sharpless and Meldal in the early 2000s, is a foundational example of click chemistry, known for its efficiency, reliability, and biocompatibility **[5]**.

Triazole derivatives exhibit a broad spectrum of biological activities, including antifungal, antibacterial, anticancer, antiviral, and anti-inflammatory effects **[6, 7]**. Several triazole-containing drugs, such as fluconazole, itraconazole, and voriconazole, are clinically approved antifungal agents targeting ergosterol biosynthesis in fungal cell membranes **[8]**. Beyond pharmaceuticals, triazoles also find applications in agrochemicals, dyes, corrosion inhibitors, and as ligands in coordination chemistry **[9]**.

Due to their wide-ranging applications and favorable properties—such as metabolic stability, hydrogen bonding capabilities, and resistance to hydrolysis—triazoles continue to be a focus of extensive research in chemical and biological sciences.

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In the presence study, we have synthesized substituted 1,2,4-triazoles by refluxing chalcones with 4H-1,2,4-trizoles-3-amine in the presence of NaOH under ethanol solvent. All the synthesized compounds were characterized using spectroscopic techniques and tested for their antimicrobial activity against gram +ve and gram -ve bacteria.

METHODS AND MATERIALS

Chemicals and Reagents

All the chemicals such as aromatic aldehyde, 4H-1,2,4-triazoles-3-amine, cyanuric chloride, sodium hydroxide, and ethanol etc. are reagent-grade and were used direct without further purification as received from Merck, Mumbai, India

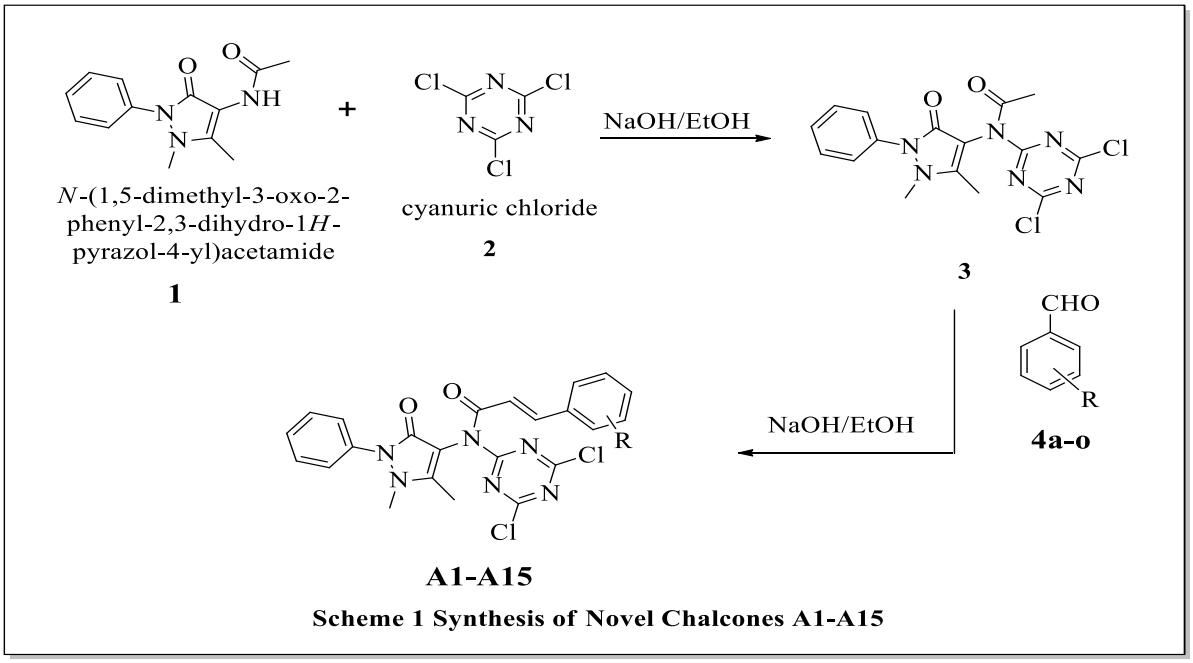
Experimental

For the ^{1}HNMR investigation, a Bruker Avance-400 instrument was used and for the ^{13}CNMR study, a 100MHZ frequency equipment. Chemical shift value was reported in parts per million. The infrared spectrum analysis was conducted using FT-IR 3000 Spectrophotometer from ABB Bomem Inc. The measured data were expressed in cm^{-1} units. For MASS spectrum analysis, Shimadzu LCMS-2010 was used.

Method of Synthesis

Synthesis of chalcones A1-A15

To a solution of N-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)acetamide compound contain heterocycle along with acetyl group **1** (0.01 mol) is taken in absolute ethanol (40 ml), add 2% NaOH and Cyanuric chloride **2** (0.01 mol) and refluxed for 30 minutes to obtained product **3** then add aromatic aldehyde **4a-o** (0.01 mol) and further refluxed the mixture for 3-4hr, cooled and poured into ice cold water. The solid thus obtained was filtered and give wash of distilled water and further crystallization is done using ethanol. Products obtained called chalcones A1-A15 (**Scheme 1**).



Scheme 1 Synthesis of Novel Chalcones A1-A15

Synthesis of Triazoles B1-B15

Take Chalcone A1 (0.01 mol) in 250 ml RBF, add 0.01 mol 4H-1,2,4-triazoles-3-amine, 20 ml ethanol and 40 ml 10ml 2% NaOH. Reflux the entire mixture for 1-2 hour to produced triazoles. Completion of reaction was monitored by TLC (**Scheme 2**).

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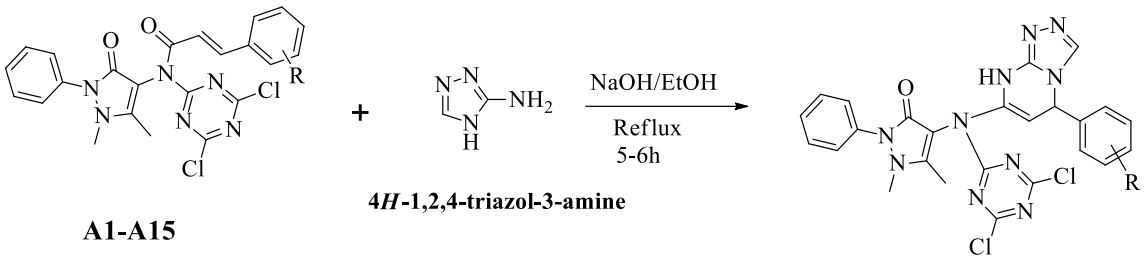

Scheme 2 Synthesis of Novel 1,2,4-triazoles B1-B15

RESULT AND DISCUSSION

Table 1 Data showing synthesis of 1,2,4-Triazoles B1-B15.

Sr. No.	Compounds Code	R	Reaction Time[a]	% Yield[b]	Melting Point (°C)
1	**B1**	-H	1.5	81	236
2	**B2**	2-OH	1.5	75	210
3	**B3**	3-OH	1.5	78	215
4	**B4**	4-OH	1.5	70	250
5	**B5**	2-Cl	2.0	85	242
6	**B6**	3-Cl	2.0	82	232
7	**B7**	4-Cl	1.5	85	227
8	**B8**	2-Br	1.5	84	215
9	**B9**	3-Br	1.5	78	240
10	**B10**	4-Br	1.5	80	221
11	**B11**	2-NO_2	1.5	84	245
12	**B12**	3-NO_2	1.5	82	257
13	**B13**	4-NO_2	1.5	84	239
14	**B14**	2-OCH3	1.5	75	213
15	**B15**	4-OCH3	1.5	76	225

[a]Reaction monitored by TLC. [b]Isolated yield

Table 1 shows the various condensation product of reaction between various chalcones with 4h-1,2,4-triazole-3amine. It clearly indicates that the compounds bearing electron withdrawing group are synthesized in shorter reaction time as compared to compounds bearing electron donating group. Compounds **B7-B15** bearing electron

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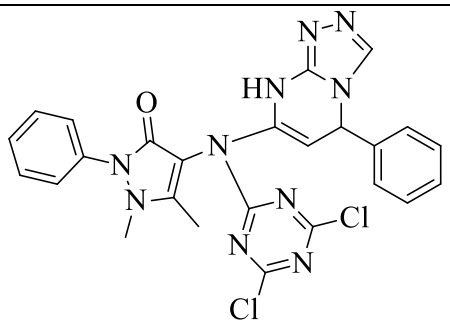
withdrawing were synthesized in **1.5hr** as compared to compounds bearing electron donating group. Compounds **B5** and **B6** having electron donating group synthesized in **2h**r.

Characterization

Compound 5a of the series is taken as the representative compound. In the ^{1}H NMR spectrum the characteristic signals due to each protons and functional groups with protons are well described on the basis of shielding and deshielding effects. The signal due to aromatic proton of compound was observed in more downfield region at chemical shift value around 6.5 to 8.4 ppm. ^{1}HNMR, ^{13}CNMR, IR, MASS spectroscopic data of compound 5a shown below.

Compound code: B1	
Molecular formula: $C_{25}H_{20}Cl_2N_{10}O$	
M. P. (°C):	**236**
^{1}HNMR (400 MHz, $CDCl_3$) **δ ppm:**	1.8 (1H, -CH, d), 2.5 (3H, -CH_3, s), 3.6 (3H, -CH_3, s), 4.1 (1H, -CH, s), 5.1 (1H, -CH, d), 6.5-8.5 (10, Ar-H), 9.1 (1H, -NH, s),.
^{13}CNMR (100 MHz, $CDCl_3$) δ ppm:	38.3, 41.3, 60.2, 68.3, 121.4, 123.2, 125.4, 128.1, 129.3, 130.3, 131.6, 134.4, 139.5, 139.9, 140.3, 142.0, 150.1, 152.0, 153.9, 185.5.
IR cm^{-1} (KBr):	3330 (N-H stretch.), 3150-3013 (Ar C-H), 2990-2915 (C-H aliphatic), 1665 (C=O), 1620 (C=C), 1594 (C=C), 1554 (C=C), 1535 (C=N), 1331 (C-N), 820 (monosubstituted phenyl ring).
Mass (M+1):	546.2
Elemental analysis:	**Calculated (%):** C, 54.85; H, 3.68; N, 25.59 **Found (%) :**C, 54.80; H, 3.62; N, 25.55

Antimicrobial Activity

Preparation of Media:

For bacterial activity nutrient agar is used. Nutrient agar is prepared as follows:

5gm Peptone, 3gm Meat Extract, 5gm NaCl and 15gm Agar-Agar Peptone were mixed in one liter distilled water and heated to dissolve all the ingredients. The medium was stabilized in autoclave at 15 pound pressure at 125^{o}C for 20 minutes. The medium was cooled down to 45^{o}C and 20 ml poured in sterilized Petri-dish. The pH of the medium was adjusted between 7.0 to 7.5. The culture of the above organism was prepared in nutrient broth dissolved in distilled water. The content of nutrient broth is:

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Beef extract : 10 gm, 2) Peptone : 10 gm 3) Sodium chloride : 5 gm

After sterilizing the above media, it was used for the culture purpose. The culture was ground at 37ºC in incubator. With the help of swab, the culture was spread over the agar plates, under specific condition 5 mm diameter paper discs were prepared and were sterilized in autoclave. The solution of the test compound was kept over these paper discs with the help of micropipette. These discs were dried to remove the solvent. Sterile test compound coated by discs were kept in Petri dish containing culture media. The discus was pressed to sterile on media and Petri dishes were incubated for 24 hours at 37ºC. After the incubations the zone of inhibition was measured.

Table 2 Experimental data of Compounds B1-B15

Samples	***S.aureus*** **(+Ve)**	***B.megaterium*** **(+Ve)**	***E.coli*** **(-Ve)**	***P.vulgaris*** **(-Ve)**
B1	10	12	12	6
B2	4	10	5	8
B3	7	6	7	3
B4	6	7	6	10
B5	10	4	3	9
B6	3	5	11	8
B7	6	10	6	9
B8	6	12	6	11
B9	7	7	9	9
B10	8	8	11	9
B11	6	4	4	11
B12	6	8	5	10
B13	9	4	7	8
B14	4	9	9	8
B15	9	12	7	9
Ampicillin	**17**	10	**15**	**14**
Gentamycin	**14**	**16**	**16**	**15**

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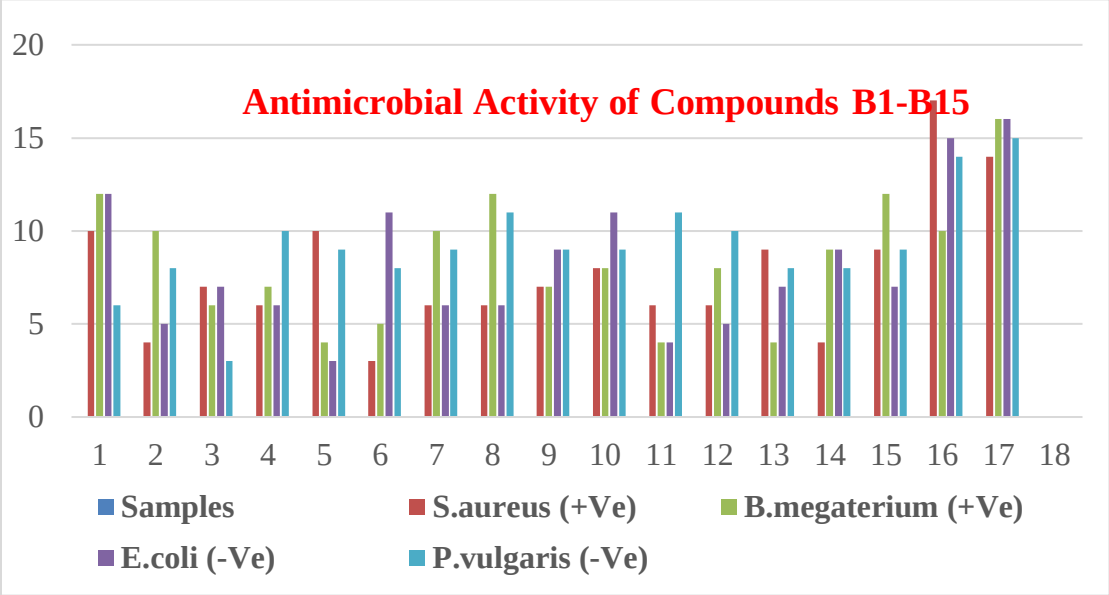

Figure 1 Antimicrobial Activity of B1-B15

CONCLUSION

In conclusion, we have synthesized highly functionalized substituted 1,2,4-triazoles from chalcones and 4H-1,2,4-triazole-3amine. It concludes that compounds such as B1, B6, B8, B10 and B15 shows good antimicrobial activity. All produced compounds were identified using various spectroscopic methods.

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