

SYNTHESIS, CHARACTERIZATION, AND ANTIBACTERIAL ACTIVITY OF NEW SATURATED HETEROCYCLIC NITROGEN COMPOUND

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Introduction and Objective: Hexahydrotriazines are concerned with a large range of six-membered ring compounds which contain three nitrogen atoms in 1,3 and 5 positions [1]. Throughout the years a considerable attraction has been obtained to hexahydrotriazines. Among various interests, the use of these kinds of products that exist in industrial chemistry. For instance, N,N',N''-trisubstituted 1,3,5-triazinanes can be used as reactants for the preparation of N-heterocyclic carbenes which served as substantial class of ligands in homogeneous catalysis their use as inhibitors for anti-corrosion activity [2]. TAC can be employed as ligand for new complexes worked as catalyst in the polymerization and trimerization of olefins. Antibiotic resistance is a major problem in hospitals as well as in community settings. Considering the ever growing antibiotic resistance developed by many bacteria, there is an immense need for new compounds with new mode of actions, for treatment of bacterial infections. The need for new antibiotics continues to be a still standing challenge. For this reason, our scientific research team has focused on this aspect through the various research published recently in many articles, which confirmed that 1,3,5-Triazacyclohexanes containing halides exhibit high biological activity against the strains of microorganisms used. since they contain CN group and halogen atom as pharmacophore. As shown by some of the results obtained: *Staphylococcus aureus* is sensitive against 1,3-bis-butyl-5-(4-iodophenyl)-1,3,5-triazacyclohexane, while resistant *Staphylococcus aureus* and *Escherichia coli* are extremely sensitive against our compound [3], *Staphylococcus aureus* is sensitive against 1,3-bis(4-iodophenyl)-5-(2-ethyl-1-hexyl)-1,3,5-triazacyclohexane and 1,3-bis(2-ethyl-1-hexyl)-5-(iodophenyl)-1,3,5-triazacyclohexane, while resistant *S. aureus* and *E. coli* are extremely sensitive against our compounds. From these results can be considered that antimicrobial activity is one of the most important applications that characterize these compounds. In the present research work, the new unsymmetrically substituted 1,3,5-triazacyclohexane was synthesized and its structure was confirmed and characterized by using various spectral techniques like FT-IR, ¹H NMR and ¹³C NMR. This compound was targeted for their antibacterial activity against Gram-positive and Gram-negative bacteria by the diffusion method on agar medium.



Methodology (Materials and methods):

An excess of formalin (37%, 30 mmol) was added dropwise to a mixture of (1:2) stoichiometric ratio of hexylamine (10 mmol, 1.32ml) and 4-chloroaniline (20 mmol, 2.4415g) which is dissolved in 25 ml of ethanol in a simple necked round bottomed flask and stirred for 12h (overnight) at 20 °C. The resulting solution was evaporated in a rotary evaporator to dryness and the white residue was recrystallized from n-hexane to afford 3,5-bis (4-chlorophenyl) - 1- hexyl-1, 3, 5-Triazacyclohexane, this compound is stable at room temperature and obtained in high yield 71%. The final obtained result was transparent colorless plaques

Results and Discussion

1/ IR spectrum interpretation: 3050 (νC-H, Ar-H), 2964 (CH₃, CH₂), 1249 (C≡N), 819 (C-Cl), 727 (δCH,Ar).

2/ Interpretation of ¹H NMR spectrum: ¹H- NMR (400 MHz, CDCl₃, δ ppm):3.38 (s, 6H, Ar-N-CH₂-Ar); 3.62 (s, 6H, Ar-N-CH₂-N-Ar); 7.21-7.33 (m, 12H, Ar).

3/ Interpretation of ¹³C NMR spectrum:

¹³C- NMR (100.62 MHz, CDCl₃, δ ppm): 56.17 (Ar-N-CH₂-Ar), 73.46 (Ar-N-CH₂-N-Ar); 132.84 (C-Cl); 115.16 – 128.40-130.09 (CH=C-), 132.48 (N-C=)

4/ Elementary analysis result

Table 1: results of the elementary analysis

results	% nitrogen	% carbon	% hydrogen	% sulphur
1	10.29	62.81	7.57	0.00
2	10.39	63.24	7.63	0.00
average	10.34	63.06	7.58	0.00
theory	10.76	70.56	7.05	0.00

5/ X-ray diffraction results

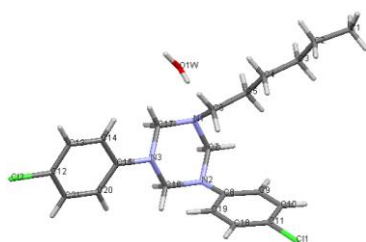


figure.1: Asymmetric unity

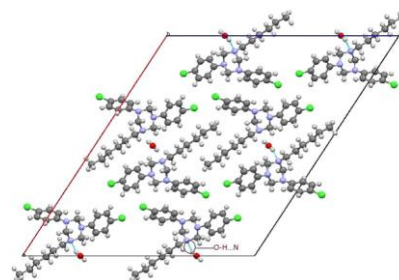


figure.2: Projection of the structure on the

6/ Antibacterial activity results

Table 2: Antibacterial activity of 3,5-bis (4-chlorophenyl) - 1- hexyl-1, 3, 5- Triazacyclohexane

The microbial strains	Concentrations				
	100	250	500	750	1000
<i>E. coli</i>	/	/	8	10	12
<i>P. aeruginosa</i>	/	/	/	/	/
<i>S. aureus</i>	13	15	10	12	/

Conclusion: In this manuscript, we have described the synthesis of a new triazacyclohexanes (R3TAC) derivative by the condensation reaction of a 2:1 mixture of 4-chloroaniline and hexylamine with formalin in ethanol . the synthesized compounds was obtained with good yield, was recrystallised with hexane. The structure of the synthesized compound was confirmed and characterized by using various spectral techniques like FT-IR, ¹H NMR, ¹³C NMR, UV, X-ray diffraction and elementary analysis. The compound was targeted for their antibacterial activity against Gram positive and Gram negative bacteria by the diffusion method on agar medium.

Keywords: Synthesis, Amine, Hexahydrotriazines, Characterization, Antimicrobial activity.

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