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Spectroscopic Investigation and Synthesis of N-Ethyl-5-Tolyloxymethyl Triazole Derivatives

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ABSTRACT

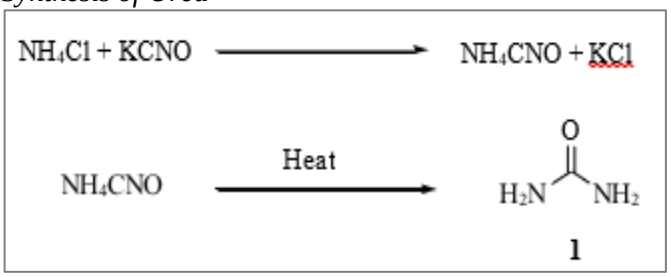
High-nitrogen heterocycles' synthesis has attracted much interest because of their wide applicability in many different sectors. As a significant class of organic compounds, triazoles and their fused derivatives have emerged among these. A new triazole derivative, 4-ethyl-3-ethylthio-5-(p-tolyloxymethyl)-4H-1, 2, 4-triazole, is the subject of this work on synthesis and spectrum characterization. Ethyl 2-p-tolyloxy acetate is synthesized by reacting 3, 4-dimethoxyphenylacetic acid with ethanol under concentrated H2SO4, starting the process. The ester product is subsequently transformed into 2-p-tolyloxyacetohydrazide, which is further reacted with ethyl isothiocyanate to produce 2-p-tolyloxythiosemicarbazide. Cyclizing 275 in an alkaline media generates 4-ethyl-5-(p-tolyloxymethyl)-4H-1, 2, 4-triazole-3-thiol. 276 interacts with several alkyl halides in the last stage to create N-ethyl-3, 5-substituted derivatives (278a-h). Infrared (IR), nuclear magnetic resonance (NMR), electron ionization mass spectrometry (EI-MS), and high-resolution electron ionization mass spectrometry (HR-EI-MS) were used to characterize each chemical. This work adds to the expanding area of nitrogen-rich heterocycles by providing fresh triazole derivatives with possible uses in industrial and medical chemistry.

INTRODUCTION

Many industrial uses and biological activities depend on organic molecules, especially heterocyclic ones. Particularly in the synthesis of novel organic compounds, the early twenty-first century saw a notable advance in the area of organic chemistry (Abdelrehim et al., 2021). Among these, heterocyclic compounds especially triazoles have become more important because of their various biological activities and wide variety of industrial uses (Almasirad et al., 2011). Depending on the location of nitrogen atoms inside the five-membered ring, triazoles show notable isomerism. Widely employed as fungicides, plant retardants, and antibacterial agents, their significance in medicinal chemistry cannot be emphasized. (Almulla et al., 2017) .

Over the years, organic chemistry has developed with revolutionary discoveries. The creation of organic chemicals like the alizarin dye in 1869 by Lieberman and the synthesis of indigo dye in 1963, for example, provided fresh possibilities for their use in textiles, medicine, and industry (Arora et al., 2012). Friedrich Wohler created one of the first discoveries in organic chemistry in 1828 by synthesizing urea from ammonium cyanate, according to Asif et al. (2015). This turning point raised the importance of organic chemistry as a central scientific discipline and set in motion findings with significant consequences for the health, pharmaceutical, and agricultural sectors (Ata et al., 2022).

Figure 1
Synthesis of Urea



The finding of several organic chemicals with therapeutic uses was especially remarkable in organic chemistry. For example, the isolation of penicillin in 1928 transformed medicine; next came the manufacture of morphine-like drugs for pain management (Campos et al., 2009). Organic compounds are also very important in the fight against infectious diseases. Antimicrobial and antibacterial drugs made from organic molecules are very important (Cansız et al., 2004).

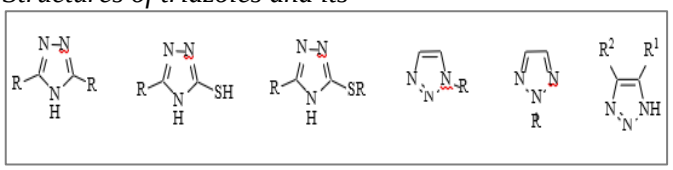
Triazoles have become a particularly significant class within the field of heterocyclic chemistry as a result of their biological activity and adaptability (Colanceska-Ragenovic et al., 2001). Especially 1, 2, 4-triazole derivatives have shown potential as antifungal, antibacterial, hypnotic, anticancer, anti-inflammatory, and anti-diabetic drugs. As a result, medicinal chemistry has been a key focus of study on the synthesis and creation of triazole derivatives (Dastjerdi et al., 2020). Many different types of illnesses, such as cancer, bacterial infections, and neurological disorders, have been studied by synthesizing and testing triazole-based drugs (Dehestani et al., 2018).

Triazoles' biological activity is due to their capacity to interact with important enzymes and receptors in the body, which results in therapeutic effects (Desai et al., 2012). For instance, certain triazoles possess potent anticancer properties by inhibiting tumour growth, while others have demonstrated significant potential in the treatment of infectious diseases, including tuberculosis and malaria (Dugdu et al., 2014). The potential of triazoles as valuable agents in the struggle against a variety of health challenges is underscored by the expanding body of research on them (Gupta et al., 2012).

Furthermore, the creation of triazole-based molecules is not restricted to their therapeutic uses (Hameed et al., 2014). In agricultural chemistry, where they are employed as herbicides and pesticides to protect crops from diseases and pests, these chemicals also have significant influence (Hasan et al., 2011). Triazoles are very useful in many different fields, so they are used in both medicine and farming (Hussain et al., 2008).

The synthesis of new triazole compounds and their biological activity is the main emphasis of this research. This work adds to the ongoing study on making new compounds that are more effective as medicines by looking into how to make 4-ethyl-3-ethylthio-5-(p-tolyloxymethyl)-4H-1,2,4- triazole and its derivatives. The structures and biological activity of the compounds synthesised in this work were confirmed through the use of multiple analytical techniques, such as mass spectrometry (MS), infrared (IR) spectroscopy, and nuclear magnetic resonance (NMR) spectroscopy (Kalhor et al., 2015).

Figure 2
Structures of triazoles and its



Triazole derivative synthesis is a promising frontier in the development of novel agrochemicals and pharmaceuticals (Kapriet al., 2020). With the possibility to provide creative answers to certain of the most urgent health and environmental concerns, this study contributes to the expanding body of information on the function of triazoles in medicine and agriculture. (Khanage et al., 2013).

LITERATURE REVIEW

In medicinal chemistry, heterocyclic compounds, particularly those that contain nitrogen atoms, are a critical category of organic compounds (Kidwai et al., 2002). Usually, carbon and heteroatoms like nitrogen, oxygen, or sulphur define these compounds' closed-chain structure with at least two distinct atoms (Kumudha et al., 2013). A subfamily of heterocyclic compounds, triazoles are made up of a five-membered ring containing three nitrogen atoms and two carbon atoms. Because of their biological activity and structural plasticity, triazoles and their derivatives are widely used in the pharmaceutical industry for a variety of therapeutic purposes, including antibacterial, anticancer, anti-inflammatory, and antifungal medicines.

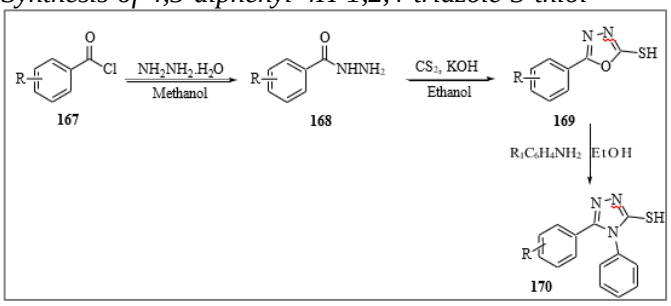
Triazoles have been extensively studied for their therapeutic properties. The development of new antibiotic drugs has been driven by the increasing resistance of microorganisms to current antibiotics. Research on triazoles is crucial because of their moderate to outstanding antibacterial qualities, especially those of 1, 2, 4-triazole derivatives (Mahdi et al., 2017). For example, recent research has demonstrated that numerous 1, 2, 4-triazole derivatives possess significant antibacterial activity against prevalent bacterial pathogens, underscoring their potential as novel antibiotic choices (Malani et al., 2016).

Synthesis of 1, 2, 4-Triazoles

An extensive body of research has been conducted on the synthesis of 1, 2, 4-triazoles and their derivatives, and a

variety of synthetic routes have been developed over the years. It is common to use modified benzoic acids to cyclize thiocarohydrazide (Li et al., 2012). This reaction results in the formation of 4-amino-5-(substituted phenyl)-4H-1, 2, 4-triazole-3-thiol, that can be further developed by condensation with aromatic aldehydes to produce triazole derivatives with improved biological activity (Prachand et al., 2018).

Figure 3
Synthesis of 4,5-diphenyl-4H-1,2,4-triazole-3-thiol



Similarly, isonicotinic acid hydrazide has been combined with carbon disulphide to form 4-amino-5-pyridin-4-yl-4H-1, 2, 4-triazole-3-thiol, a molecule with antibacterial properties (Nadeem et al., 2013). Mannish base derivatives were generated through additional modifications that included primary or secondary amines and aromatic aldehydes, which also demonstrated substantial microbial activity (Bayrak et al., 2009).

Another synthesis approach involves reacting phenylacetic acid hydrazide with carbon disulphide in an ethanolic potassium hydroxide solution, then reacting with hydrazine hydrate to produce triazole derivatives (Maji et al., 2018). This method is a highly efficient approach to the synthesis of a diverse array of 1, 2, 4-triazoles, which are subsequently evaluated for their antimicrobial and anticancer properties (Cansız et al., 2004).

Furthermore, substituted aromatic acids can be esterified with methanol in the presence of strong sulphuric acid to produce the appropriate esters (Nanjan et al., 2018). Hydrazide derivatives can be produced by condensation of these esters with hydrazine hydrate. Upon cyclisation, these derivatives can be converted to triazoles that possess potential medicinal benefits (Singh et al., 2009).

Biological Activities of Triazoles

Triazoles have attracted notice for their several biological activities (Patel et al., 2021). They have been made as anticonvulsants, and some of their derivatives have been shown to effectively control seizures (Dehestani et al., 2018). Furthermore, triazoles are notable anticancer drugs since research show they can prevent tumour growth and metastasis, thereby qualifying them for cancer treatment (Singh et al., 2012). Triazoles, in addition to their anticancer effects, include antimicrobial activities such as antibacterial, antifungal, and antiviral capabilities, which contribute to their use in the treatment of various illnesses (Shukla et al., 2014).

Moreover, triazoles have been found to be efficient antidiabetic drugs, especially in the shape of thiazolidinedione derivatives, which are utilised to control Type 2 diabetes (Hossein et al., 2020). Their capacity to affect glucose metabolism has drawn much study for the creation of novel antidiabetic drugs (Pertino et al., 2017). Furthermore, triazoles have showed potential as antimalarial medicines, with molecules demonstrating in vitro and in vivo efficacy against Plasmodium falciparum, the malaria-causing parasite (Singh et al. 2010).

Moreover, one important quality of triazole derivatives is anti-inflammatory action; certain molecules show considerable efficacy in lowering pain and inflammation (Saini et al., 2013). Tested in several animal models, these substances show promise for treating conditions including arthritis and other inflammatory diseases (Pertino et al., 2017).

The various biological actions of triazoles make them main contenders for pharmaceutical development. Their inclusion into medicinal chemistry offers great potential for the development of new, strong therapies (Zhang et al., 2017). Additionally, the increasing interest in sustainable agriculture has resulted in the investigation of triazole derivatives as pesticides and herbicides, providing solutions to effectively control pests and increase crop yields (Sahoo et al., 2010).

Future investigations are anticipated to concentrate on optimizing the pharmacological profiles of triazole-based drugs, improving their selectivity, and minimizing adverse effects as research on these molecules advances. Researchers are still coming up with new ways to make triazole derivatives. This will lead to a wider range of chemicals that could help treat infectious diseases, cancer, and other long-term illnesses.

MATERIALS AND METHODOLOGY

Chemical Reagents

Analytical grade chemicals were utilized to synthesize compounds 278a-h. Sigma-Aldrich supplied various alkyl halides as well as ethyl isothiocyanate. E. Merck supplied hydrazine hydrate. The following chemicals were purchased from nearby vendors: NaOH, KOH, chloroform, CCl_4, methanol, ethanol, n-hexane, ethyl acetate, sulphuric acid, hydrochloric acid, and sodium carbonate.

Purification of Solvents

Alcohols, n-hexane, ethyl acetate, methanol, and other liquids were distilled before they were used to make sure they were as pure as possible.

Instrumentation

The 13C-NMR spectra were taken with the same

instrument, but this time set to 100 MHz and using TMS as the internal standard. The 1H-NMR spectra were recorded on a Bruker analyser working at 400 MHz. The chemical changes (δ) were measured in ppm. There were four types of signal multiplicities: singlet (s), triplet (t), quartet (q), and multiplet (m). IR spectra were recorded with an FTIR spectrometer from Shimadzu (model 460). A JMSA 500 mass analyser was used for the mass spectrometry. An electrothermal device made by Gallen Kemp was used to find the melting points.

Synthesis of Ethyl 2-(p-tolyloxy) acetate (273)

Ethyl 2-(p-tolyloxy) acetate (273) was synthesised by continual stirring of ethanol with 0.4 g of 4-methylphenoxyacetic acid added to it. Four hours of refluxing were applied to the reaction mixture. The product was collected after the reaction, resulting in the isolation of ethyl 2-(p-tolyloxy) acetate as a colourless liquid with a boiling point of 90-92˚C and a yield of 90%. The spectroscopic information of the compound is as follows:

- IR (KBr, υmax, cm-1): 3036 (Ar-H), 2945 (C-H), 1725, 1657 (C=O), 1614-1554 (Ar-C=C), 1256 (C-O)
- 1H-NMR (400 MHz, $CDCl_3$, ppm): δ 1.23 (3H, t, J = 6.8 Hz, CH_3-CH_2-O), 2.40 (3H, s, CH_3-Ph), 4.19 (2H, q, J = 6.8 Hz, CH_3-CH_2-O), 4.95 (2H, s, H-2a), 7.00 (2H, d, J = 8.5 Hz, H-2′,6′), 7.30 (2H, d, J = 8.5 Hz, H-3′,5′)
- 13C-NMR (100 MHz, $CDCl_3$, ppm): δ 13.4 (O-CH_2-CH_3), 21.5 (CH_3-Ph), 65.1 (C-2a), 63.2 (O-CH_2-CH_3), 115.0 (C-2′,6′), 129.0 (C-3′,5′), 131.0 (C-4′), 151.1 (C-1′), 165.9 (C=O)
- HR-EI-MS (m/z): 180.0786 [M] +, calculated for $C_{10}H_{12}O_3$, 180.0779.

Synthesis of 2-p-tolyloxyaceto hydrazide (274)

In a round-bottom flask that contained 30 ml of hydrazine hydrate, 1.4 g of ethyl 2-p-tolyloxyacetate (273) was added to synthesise 2-p-tolyloxyaceto hydrazide (274). TLC monitored the reaction mixture for four hours and stirred it until it was complete. The white, shiny powder that was made had a melting point of 150–152˚C and an output of 92%. The compound's spectroscopic data is as follows:

- IR (KBr, υmax, cm-1): 3392, 3356 (N-H), 3036 (Ar-H), 2947 (C-H), 1720, 1655 (C=O), 1610-1556 (Ar-C=C), 1253 (C-O)
- 1H-NMR (400 MHz, $CDCl_3$, ppm): δ 2.26 (3H, s, CH_3-Ph), 4.64 (2H, s, H-2a), 7.00 (2H, d, J = 8.5 Hz, H-2′,6′), 7.20 (2H, d, J = 8.5 Hz, H-3′,5′)
- 13C-NMR (100 MHz, $CDCl_3$, ppm): δ 20.9 (CH_3-Ph), 66.3 (C-2a), 115.8 (C-2′,6′), 130.0 (C-3′,5′), 131.9 (C-4′), 155.1 (C-1′), 166 (C=O)
- HR-EI-MS (m/z): 166.0742 [M]+, calculated for $C_8H_{10}N_2O_2$, 167.0739.

Synthesis of 2-(p-tolyloxymethylcarbonyl) thiosemicarbazide (275)

The synthesis of 2-(p-tolyloxymethylcarbonyl)thiosemicarbazide (275) was achieved by combining 1.5 g of p-tolylacetohydrazide (274) with 0.5 ml of ethyl isothiocyanate in a round-bottom flask. For four to five hours, the mixture was refluxed and agitated. A white solid with a melting point of 180-182˚C and a yield of 90% was extracted from the precipitates of the product. As follows is the compound's spectroscopic data:

- IR (KBr, υmax, cm-1): 3390, 3354 (N-H), 3033 (Ar-H), 2950 (C-H), 1690, 1658 (C=O), 1613-1557 (Ar-C=C), 1245 (C-O)
- 1H-NMR (400 MHz, $CDCl_3$, ppm): δ 1.27 (3H, t, J = 7.2 Hz, CH_3-CH_2-NH), 2.22 (3H, s, CH_3-Ph), 4.36 (2H, q, J = 7.0 Hz, CH_3-CH_2-NH), 4.71 (2H, s, H-2a), 7.30 (2H, d, J = 8.5 Hz, H-2′,6′), 7.40 (2H, d, J = 8.5 Hz, H-3′,5′)
- 13C-NMR (100 MHz, $CDCl_3$, ppm): δ 15.4 (CH_3-CH_2-NH), 21.2 (CH_3-Ph), 39.8 (CH_3-CH_2-NH), 116.2 (C-2′,6′), 129.4 (C-3′,5′), 131.7 (C-4′), 154.2 (C-1′), 165.2 (C=O), 183.9 (C=S)
- HR-EI-MS (m/z): 253.0885 [M]+, calculated for $C_{11}H_{15}N_3O_2S$, 253.0879.

Synthesis of 4-Ethyl-5-(p-tolyloxymethyl)-4H-1,2,4-triazole-3-thiol (276)

In a round-bottom flask, 2.1 g of p-tolyl 2-(ethylcarbamothioyl) hydrazine-1-carboxylate (275) was mixed with a 1% NaOH solution to make 4-ethyl-5-(p-tolyloxymethyl)-4H-1,2,4-triazole-3-thiol (276). Concentrated hydrochloric acid was added to the product after the combination had refluxed for four hours under TLC monitoring. There was a 91% yield and a melting point of 211-214˚C for the 276 precipitates that were gathered. They were a white, amorphous solid. The compound's spectroscopic information is as follows:

- IR (KBr, υmax, cm-1): 3034 (Ar-H), 2930 (C-H), 1617-1551 (Ar-C=C, C=C), 1227 (C-N), 1247 (C-O)
- 1H-NMR (400 MHz, $CDCl_3$, ppm): δ 1.29 (3H, t, J = 7.2 Hz, CH_3-CH_2-NH), 2.24 (3H, s, CH_3-Ph), 4.21 (2H, q, J = 7.0 Hz, CH_3-CH_2-NH), 5.31 (2H, s, H-5a), 7.00 (2H, d, J = 8.5 Hz, H-2′,6′), 7.01 (2H, d, J = 8.5 Hz, H-3′,5′)
- 13C-NMR (100 MHz, $CDCl_3$, ppm): δ 13.8 (CH_3-CH_2-N), 21.1 (CH_3-Ph), 31.8 (CH_3-CH_2-N), 68.9 (C-5a), 116.4 (C-2′,6′), 129.9 (C-3′,5′), 130.9 (C-4′), 157.0 (C-1′), 158.2 (C-3), 164.5 (C-5)
- HR-EI-MS (m/z): 249.0936 [M]+, calculated for $C_{12}H_{15}N_3OS$, 249.0929.

RESULTS AND DISCUSSION

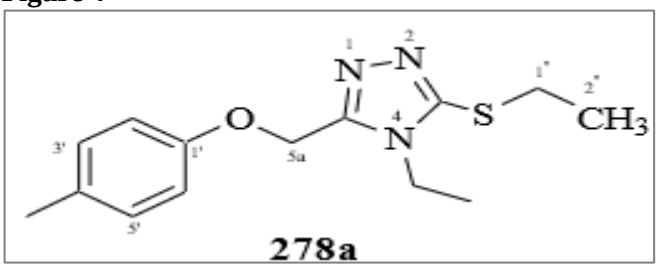
Specifically meant to investigate the biological activity and chemical properties of 1,2,4-triazoles, the

synthesised molecules 278a-h are a series of unique triazole derivatives. Synthesis of these compounds in high yields and characterisation by many spectroscopic techniques—including IR spectroscopy, 1H-NMR, 13C-NMR, and HR-EI-MS—verified their structures and molecular formulae.

Structure Elucidation of Compound 278a

Synthesized as a white glossy powder with a melting point of 78-79ºC and a yield of 93%, compound 278a (3-ethylthio-4-ethyl-5-(p-tolyloxymethyl)-4H-1,2,4-triazole) was The IR spectrum had clear absorption lines at 3027 cm-1 (Ar-H), 2932 cm-1 (C-H), and 1619–1554 cm-1 (Ar-C=C, C=C), which showed that aromatic and aliphatic functions were present. The 1H-NMR spectrum exhibited signals that were consistent with the ethyl group attached to both sulphur and nitrogen atoms. The ethyl groups were detected as triplet and quartet signals at δ 1.35 and δ 2.98. A total of twelve signals were identified in the 13C-NMR spectrum. These signals corresponded to ethyl groups connected to sulphur and nitrogen, at δ 14.8 and δ 28.1, respectively. With a molecular ion peak at 277.1239, HR-EI-MS verified the molecular formula C14H19N3OS.

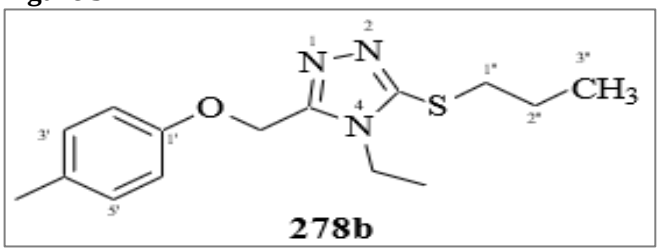
Figure 4



Structure Elucidation of Compound 278b

It was possible to get compound 278b (3-n-propylthio-4-ethyl-5-(p-tolyloxymethyl)-4H-1,2,4-triazole) as a white powder that sparkled. It melted at 75–76ºC and 91% of it was used. The IR spectrum of 278b revealed comparable absorption bands to 278a, therefore verifying the existence of comparable functional groups. The n-propyl group connected to sulphur showed triplet signals at δ 1.06 and δ 3.10 in the 1H-NMR spectrum, while the ethyl group coupled to nitrogen showed signals at δ 1.34 and δ 4.09 in the same spectrum. The structure of 278b was confirmed by the 13C-NMR spectrum, which displayed a total of thirteen signals. HR-EI-MS revealed a molecular ion peak at 291.1403, allowing the chemical formula C15H21N3OS to be calculated.

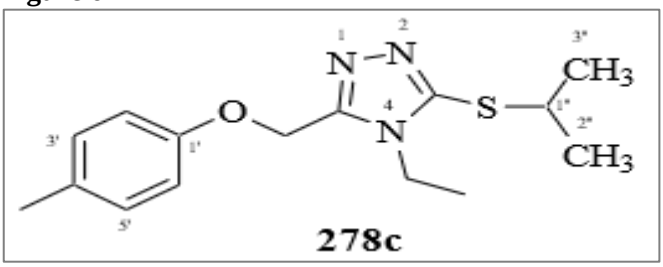
Figure 5



Structure Elucidation of Compound 278c

A white, amorphous material called 278c (3-isopropylthio-4-ethyl-5-(p-tolyloxymethyl)-4H-1,2,4-triazole) was made. Its melting point was 88–89ºC, and 90% of it was produced. The IR spectrum had bands that looked a lot like the 278a and 278b bands. A septet signal at μ 3.09 was seen in the 1H-NMR spectrum for the methine of the isopropyl group, which showed that it was attached to sulphur. Signals at \u00b4 1.32 and \u00b4 4.11 verified the ethyl group connected to nitrogen in the triazole ring. Twelve total signals on the 13C-NMR spectrum verified the isopropyl group and the ethyl group attached to nitrogen. HR-EI-MS verified the chemical formula C15H21N3OS with a molecular ion peak of 291.1401.

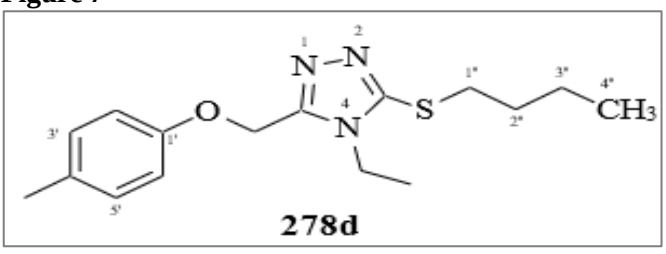
Figure 6



Structure Elucidation of Compound 278d

A white amorphous particle with a melting point of 98-99ºC and a yield of 89% was synthesized as Compound 278d (3-n-butylthio-4-ethyl-5-(p-tolyloxymethyl)-4H-1,2,4-triazole). A-H absorption bands were found at 3032 cm-1, C-H bands at 2936 cm-1, and Ar-C=C and C=C bands at 1623 and 1557 cm-1. Quintet and triplet signals were observed in the 1H-NMR spectrum, which were consistent with the n-butyl group attached to sulphur at δ 1.68, δ 1.46, and δ 3.18, as well as the ethyl group attached to nitrogen at δ 1.34 and δ4.12. The n-butyl group's presence at δ 13.8 and δ 36.3, as well as the ethyl group's presence at δ 15.8 and δ 31.3, was verified by the 13C-NMR spectrum. HR-EI-MS has verified the molecular formula C16H23N3OS, with the molecular ion peak located at 305.1559.

Figure 7

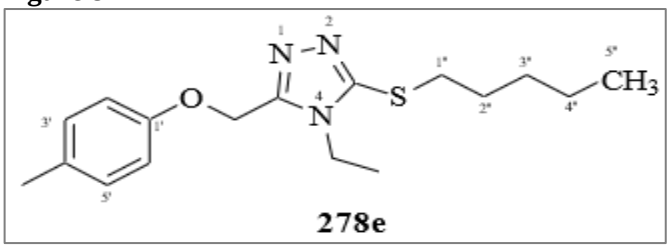


Structure Elucidation of Compound 278e

A white amorphous powder with a melting point of 85-86ºC and a yield of 92% was compound 278e (3-n-pentylthio-4-ethyl-5-(p-tolyloxymethyl)-4H-1,2,4-triazole). Typical absorption bands were observed in the IR spectrum at 3034 cm-1 (Ar-H), 2935 cm-1 (C-H), and 1617-1552 cm-1 (Ar-C=C, C=C). The 1H-NMR spectra

revealed the presence of n-pentyl groups at δ 0.94, δ 1.39, and δ 3.16, as well as an ethyl group linked to nitrogen at δ 1.34 and δ 4.09. A total of fifteen signals on the 13C-NMR spectrum confirmed the structure of 278e. HR-EI-MS validated the chemical formula C17H25N3OS, with a molecular ion peak at 319.1715.

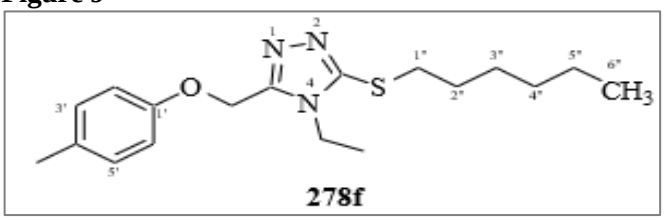
Figure 8



Structure Elucidation of Compound 278f

The synthesis of Compound 278f (3-n-hexylthio-4-ethyl-5-(p-tolyloxymethyl)-4H-1,2,4-triazole) resulted in a white, lustrous solid with a melting point of 83-84ºC and a yield of 91%. The IR spectra showed expected absorption bands for aliphatic and aromatic functional groups. The n-hexyl group was confirmed to be present at δ 1.37, δ 1.72, and δ 3.18 in the 1H-NMR spectrum, while the ethyl group was connected to nitrogen at δ 1.35 and δ 4.08. The 13C-NMR spectrum confirmed the structure of 278f by revealing sixteen signals. HR-EI-MS validated the chemical formula C18H27N3OS, with the molecular ion peak located at 333.1869.

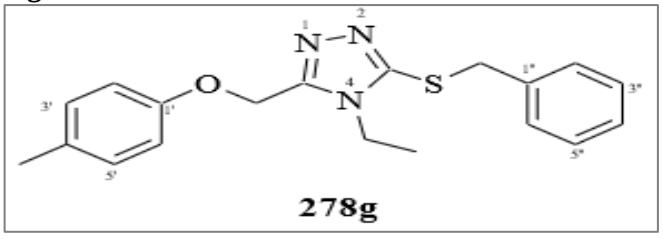
Figure 9



Structure Elucidation of Compound 278g

A white amorphous material called 278g (3-benzylthio-4-ethyl-5-(p-tolyloxymethyl)-4H-1,2,4-triazole) was made. Its melting point was 133–134o and its yield was 92%. The IR spectra revealed expected absorption bands for aromatic and aliphatic groups. The 1H-NMR spectrum showed that the benzyl group was present at ε 4.32 and μ 7.26-7.40. The 13C-NMR spectrum confirmed the structure of 278g by displaying fifteen signals for the carbon atoms. Another test called HR-EI-MS confirmed the molecular formula C19H21N3OS. The molecular ion peak was found at 339.1409.

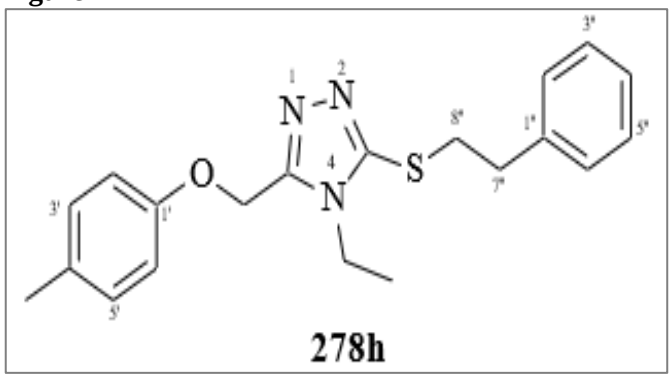
Figure 10



Structure Elucidation of Compound 278h

Compound 278h (3-phenethylthio-4-ethyl-5-(p-tolyloxymethyl)-4H-1,2,4-triazole) was synthesized as a white amorphous solid with a melting point of 148-149ºC and a yield of 95%. The IR spectrum displayed typical absorption bands for aromatic and aliphatic functional groups. The 1H-NMR spectrum confirmed the presence of the phenethyl group at δ 3.08, δ 3.44, and δ 7.17-7.40. The 13C-NMR spectrum revealed sixteen signals for the carbon atoms, confirming the structure of 278h. The molecular formula C20H23N3OS was confirmed by HR-EI-MS, with the molecular ion peak at 353.1559.

Figure 11



CONCLUSION

In this study, we successfully synthesized and characterized a series of N-ethylated 4H-1,2,4-triazole derivatives (278a-h) using a systematic approach involving alkylation reactions, hydrazine condensation, and thiol functionalization. The compounds were synthesized in high yields, with excellent purity, as confirmed by their detailed spectroscopic data including IR, NMR, and HR-EI-MS analysis. The structure elucidation of the synthesized compounds demonstrated the successful incorporation of alkyl groups and functional moieties into the triazole ring. The IR, NMR, and mass spectral data confirmed the presence of the expected functional groups, such as alkylthio, ethyl, and phenoxymethyl groups, providing strong evidence for the successful synthesis of the desired compounds. The diverse range of alkyl substituents attached to the sulfur atom of the triazole ring (ethyl, n-propyl, isopropyl, n-butyl, n-pentyl, n-hexyl, benzyl, and phenethyl) demonstrates the versatility of the synthesis method and provides a valuable set of compounds for further exploration in drug design, material science, and other applications. Future studies will focus on exploring the biological and pharmacological activities of these compounds, along with their potential as functional materials, thus expanding their utility in various scientific fields. The synthetic approach outlined herein offers a robust and scalable method for the preparation of similar N-ethylated triazole derivatives.

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