SYNTHESIS AND CHARACTERIZATION OF NEW TETRAZOLE COMPOUNDS AND STUDY OF THE BIOLOGICAL AND LASER ACTIVITY, MOLECULAR DOCKING, AND LIQUID CRYSTAL OF SOME COMPOUNDS

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Received 09.11.2025
Accepted 19.01.2026

Abstract: *Through this study, a number of new tetrazole derivatives were formed by reacting Schiff lead derivatives with NaN_3 in the presence of DMF as a solvent using an environmentally friendly and novel approach, namely microwave. These compounds were characterized by FT-IR and ^1H&^{13}C-NMR spectra, which confirmed that the synthesized ring was successful through the disappearance of the (C=O) group and the appearance of the amine group (NH_2), the azo group (N=N), and the (CH) group, which are the characteristic groups in tetrazole compounds. Compounds [E_5] and [E_8] were chosen because of their proven effectiveness against E. coli and S. aureus. The results showed that compound [E_5] was superior to standard antibiotics in inhibiting the growth of E. coli, while compound E_8 showed good activity at high concentrations where the two antibiotics were used. Laser irradiation studies also revealed a significant decrease in melting points and a change in color, indicating that the molecular structure of these derivatives is affected by photo-treatment. Computed tomography analysis of molecular docking using biotin carboxylase protein (PDB: 3jzf) showed that compound [E_5] exhibits the highest binding affinity and best stability within the active site, exhibiting low binding energies and multiple interactions, including hydrogen bonds and π interactions. Furthermore, optical analysis of compounds [E_5, E_8] using polarized microscopy revealed that compound E_5 exhibits clear phase behavior of a hexagonal columnar liquid (Col_h) followed by a vegetative (N) phase, while compound E_8 showed no liquid crystalline properties. These results confirm that the prepared tetrazole derivatives, particularly compound [E_5], are promising materials for pharmaceutical and bioactive applications, with potential for future use as highly effective antibacterial agents.*

Keywords*: tetrazole, Biological activity, laser effectiveness, molecular docking, liquid crystal.*

1. Introduction

Due to their importance in pharmacology, the topic of heterocyclic compounds has received considerable attention in recent years [1, 2]. In the fields of industrial chemistry, synthetic organic chemistry, and medicine, nitrogen-containing heterocyclic molecules appear to be particularly interesting carriers [3]. Moreover, the chemist community expects chemists to develop more sustainable and environmentally friendly chemical processes. Tetrazoles are important five-membered heterocyclic compounds, consisting of four nitrogen atoms and one carbon atom. Despite the advancements in the study of heterocyclic chemistry, applied chemistry continues to focus on the various applications of tetrazole heterocyclic compounds. Tetrazolate molecules were first synthesized by Paladin in 1855, and since then, there has been an annual increase in articles related to these compounds and their applications [4]. Because they possess a high proportion of nitrogen-nitrogen and carbon-nitrogen bonds, they require high temperatures for their synthesis. They also exhibit high resistance to shock, electrostatic discharge, and pulses due to their low carbon-hydrogen bonding content [5]. These tetrazole derivatives play a vital role in the development of numerous biologically active compounds that combat diseases caused by viruses and microorganisms [6]. In pharmaceutical chemistry, tetrazoles act as spacers and carboxylic acid substitutes [7]. They have also been used in the development of energy materials. Furthermore, tetrazoles provide an ideal framework for carrying out synthetic procedures to produce the required heterocyclic units. Additionally, tetrazole, which contains five-membered heterocyclic molecules, is a key component of a drug carrier used in the synthesis of potential anticancer drugs. Several

promising materials, including coordination compounds and natural compounds containing a tetrazole moiety, have been discovered [8]. Previous studies have also demonstrated that the tetrazole ring possesses high antibacterial activity [9].

This study aims to use alternative and environmentally friendly methods to prepare a number of nitrogen-containing compounds, namely tetrazole, by reacting Schiff bases with sodium azide to form five-membered rings and to test the effectiveness of these precursors against two different types of Gram-positive and Gram-negative bacteria. The molecular docking of some of these precursors and some of the prepared compounds was examined in order to achieve structural-functional compatibility with possible molecular binding sites. Additionally, the liquid crystal properties of some of the prepared compounds were examined, and their phase behavior was examined using phase analysis techniques.

2. Experimental part

2.1. Material: The materials under study were purchased from multinational global manufacturers such as Fluka, Aldrich, and BDH, as they were characterized by high purity.

2.2. Devices used: A 9300 electric thermocouple was used to measure temperatures. A KBr bromine disk and a Shimadzu FT-IR 8400S spectrometer with a resolution of 400–4000 cm^{1} were used. Bruker spectrometers operating at 400 MHz were used to obtain 1H and 13C NMR spectra. Ultraviolet light was used to visualize thin-layer chromatography (TLC) spots by testing them on 0.2 mm thick silica gel activated with fluorescent silica gel G. The Advanced Microbiology Research Laboratory at Tikrit University used a Rayba steam sterilizer (Spain) to sterilize the microbiological medium used in the study. In the same laboratory, a Heraeus D-63450 incubator (Germany) was used to incubate the inoculated Petri dishes used in the microbiological research.

2.3. Preparation of tetrazole derivatives [E_5-E_8]. In a ceramic beaker, 0.001 mol of Schiff base derivatives [E_1-E_4] were combined with 0.003 mol (0.2 g) of sodium azide and 10 mL of dimethyl formaldehyde (DMF) solvent. The beaker was then covered with perforated aluminum foil to allow vapor escape and heated in a microwave oven at 150 °C for 3–7 minutes [10]. The reaction was observed by TLC, and the resulting precipitate was collected, washed with distilled water, and recrystallized using tetrahydrofuran (THF) as described in Table 1.

Table 1. Tetrazole derivatives' physical characteristics

Comp.	R	Molecular Formula/ M.Wt g/mol	Color	Time (h)	M.P (^{0}C)	R*f*	Y. %
***E_5**	Br	$C_{42}H_{30}Br_3N_{15}$ / 984.52	Orange	6	263-265	0.75	53
E_6	Cl	$C_{42}H_{30}Cl_3N_{15}$ / 851.16	Brown	3	257-259	0.76	60
E_7	F	$C_{42}H_{30}F_3N_{15}$ / 801.80	Light brown	4	236-238	0.68	61
***E_8**	CH_3	$C_{45}H_{39}N_{15}$ / 789.91	White	7	244-246	0.69	57

2.4. Biological activity study. The antibacterial activity of the synthesized compounds was evaluated in the Department of Biology laboratory using one Gram-positive bacterium (*Staphylococcus aureus*) and one Gram-negative bacterium (*Escherichia coli*), which are among the most common bacteria of medical importance. Mueller–Hinton agar was prepared by dissolving 40 g of the medium in 1 L of distilled water and sterilized in an autoclave at 121 °C and 1.5 bar for 15 min. The sterilized medium was then poured into sterile Petri dishes and allowed to solidify [11-14]. Bacterial swabs were obtained from the microbiology laboratories of the Department of Life Sciences at the university. The bacterial inoculum was evenly spread over the surface of the agar plates in three directions to ensure uniform distribution of bacterial cells. The antibacterial activity was assessed using the **agar well diffusion method**. Wells of uniform diameter (6 mm) were made in the agar using a sterile cork borer. The synthesized compounds E5 and E8 were dissolved in dimethyl sulfoxide (DMSO) and tested at three different concentrations (0.1, 0.01, and 0.001 mg/mL). The dilution process was carried out by dissolving 0.1 g of each compound in 10 mL of

DMSO to obtain a stock solution of 0.1 mg/mL. Serial dilutions were then prepared by transferring 1 mL of the previous solution into 9 mL of DMSO to obtain concentrations of 0.01 and 0.001 mg/mL [15]. A fixed volume (100 µL) of each concentration was introduced into the corresponding wells. Amikacin and ciprofloxacin were used as positive control antibiotics for comparison with the synthesized compounds. The plates were incubated at 37 °C for 24 h, after which the antibacterial activity was evaluated by measuring the diameter of the inhibition zones (including the well diameter) using a centimeter ruler [16-19]. All experiments were performed in triplicate, and the inhibition zone values were expressed as the mean of three independent measurements.

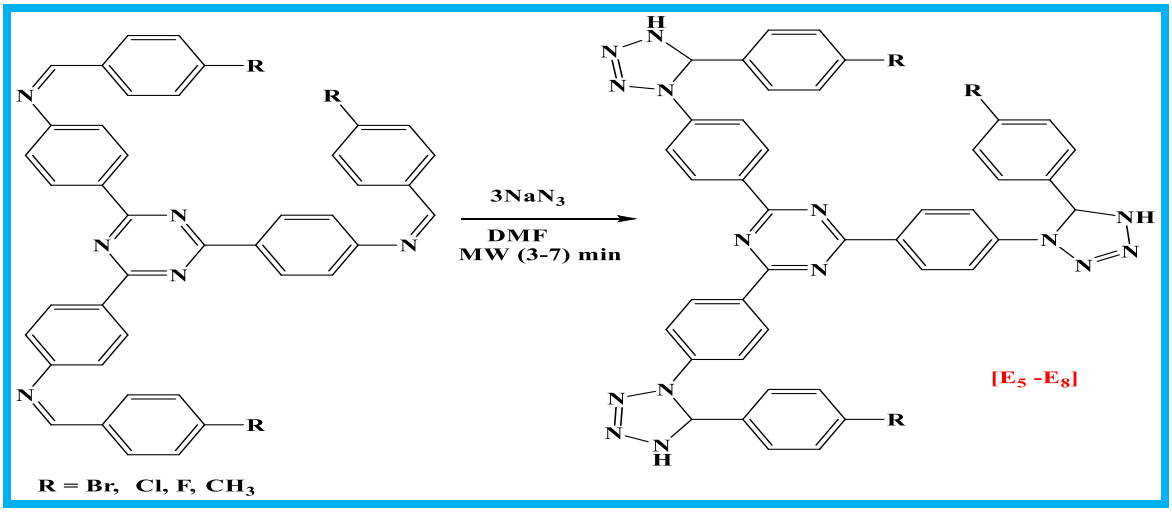
2.5. Testing the effectiveness of certain compounds against lasers. To expose the compounds [E_5, E_6, E_7, E_8] to neodymium nano-laser beams (Nd:YAG laser) with a frequency of 5 Hz and a wavelength of 808 nm. With a focal length of 100 mm, a concave quartz lens was used. The samples were exposed to laser irradiation vertically after 40 seconds of firing the laser beams at a distance of 10 cm between the laser source and the samples [20, 21].

2.6. Molecular bonding test for some compounds. Using the MOE tool (2014), molecular docking research was conducted on Escherichia coli bacteria for some synthesized compounds [E*5*, E*8*]. The proteins studied were taken from a protein bank, and the most stable configurations were found to minimize energy consumption [22]. High-performance computers equipped with fast, multi-core processors performed the complexity calculations.

2.7. Examining some produced chemicals' liquid crystal characteristics. A MEIJI high-temperature polarizing microscope, equipped with an E-PLAN 10X/0.25 160/0.17 lens and a 38-megapixel V6 high-resolution camera with 20X magnification, was used to study the texture of specific synthesized compounds [E_5, E_8]. An automated thermal imaging camera and a magnifying lens were used to precisely analyze the thin films of each chemical under investigation. The texture of the compounds was then imaged [23].

3. Results and discussion

3.1. Compounds Synthesis Scheme. Our study aimed to form a number of new compounds derived from tertiary substitution tetrazole using a new and safer method, namely microwave, by reacting at a molar ratio (1:3) of prepared Schiff bases with sodium azide, as shown in Scheme 1.



Scheme 1. Route of produced chemicals [E_5-E_8]

3.2. Characterization of tetrazole derivatives [E_5-E_8]. FT-IR analysis of the studied compounds [E_5-E_8] revealed the removal of the azomethine (C=N) band from the synthesized Schiff base, which is considered the core of the synthesis process. An extension band was found at 3336-3259 cm^{-1}, linked to (N-H) in tetrazole; an extension band at 3076-3049 cm^{-1}, linked to the aromatic (C-H) ligand; an extension band at 2937-2850 cm^{-1}, linked to the aliphatic (CH) ligand; and two extension bands at 1487-1472 cm^{-1} and 1585-1577 cm^{-1} associated with (C=C) in benzene.

An elongation band at 1444-1411 cm^{-1} is associated with (N=N) within the formed tetrazole. An elongation band at 1217-1205 cm^{-1} belonging to (C-N) [24, 25] was also found, as shown in Table 2 and Fig.s 1 and 2.

Table 2. The infrared spectral absorption values of the prepared tetrazol compounds (E_5-E_8)

Comp. No.	R	IR (KBr) cm^{-1}						
		νN-H	νC-H Arom.	νC-H Aliph.	νC=C Arom.	νN=N	νC-N	Others
E_5	Br	3276	3076	2895	1577, 1487	1423	1216	ν (C-Br) 601
E_6	Cl	3336	3049	2937	1585, 1481	1444	1207	ν (C-Cl) 700
E_7	F	3288	3055	2907	1579, 1472	1432	1205	ν (C-F) 841
E_8	CH_3	3259	3070	2850 2920	1581, 1481	1411	1215	ν (C-H) *asy.* (2920) *sym.* (2850)

Through ^{1}H-NMR of compound [E6], a multiple signal was found in the range 7.02-7.83 ppm, attributed to the benzene rings; a single signal during the displacement (5.20 ppm), attributed to the (CH) in tetrazole; a single signal during the displacement (2.16 ppm), attributed to (NH) in the same ring; and a solvent signal (DMSO-d6) was found during the displacement (2.51 ppm) (Fig. 3).

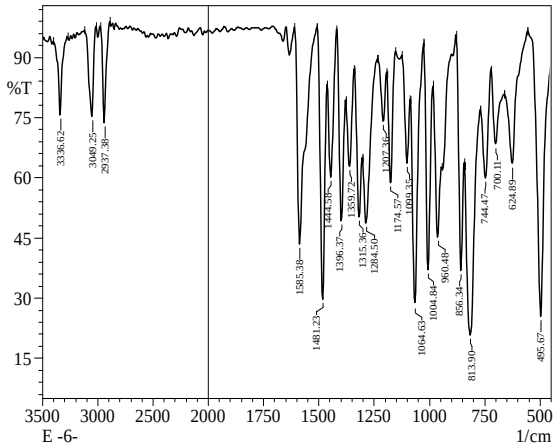


Fig 1. FT-IR spectrum for the compound E_6

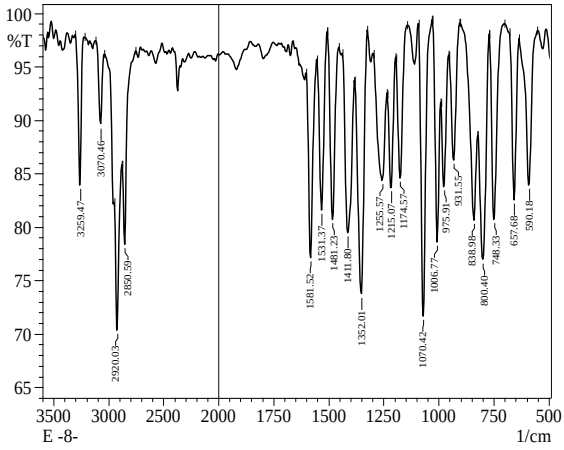


Fig 2. FT-IR spectrum for the compound E_8

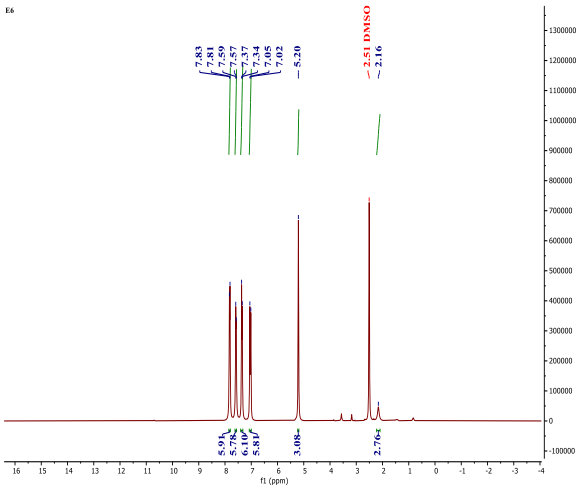


Fig 3. ^{1}H-NMR spectrum of the compound E_6

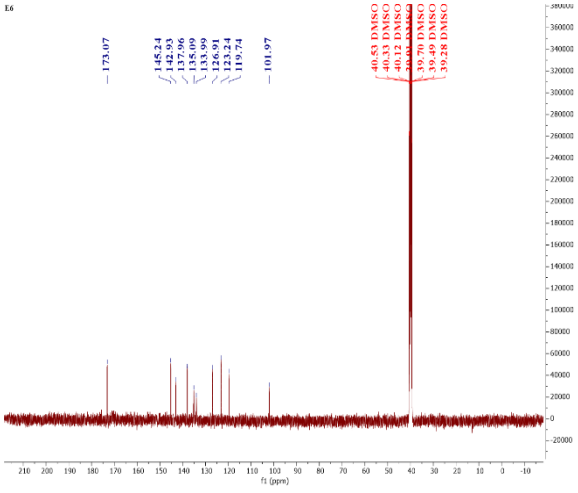


Fig 4. ^{13}C-NMR spectrum of the compound E_6

^{13}C-NMR analysis of compound [E6] revealed a signal at a displacement of 173.07 ppm associated with the triazine ring carbon, signals in the range of 119.74-145.24 ppm associated with the benzene rings, a signal at a displacement of 101.97 ppm associated with (CH) in tetrazole, and a solvent signal (DMSO-d6) found in the range of 39.28-40.53 ppm (Fig. 4).

3.3. Assessment of Prepared Compounds' Biological Activity. The antibacterial activity of the synthesized tetrazole derivatives was evaluated against Gram-negative (*Escherichia coli*) and Gram-positive (*Staphylococcus aureus*) bacteria at three concentrations, as shown in Table 3. Interestingly, compound E5 exhibited the highest inhibition zone (2.8 cm) against *E. coli* at 0.01 mg/mL**,** which is greater than that observed at the higher concentration of 0.1 mg/mL (Fig. 5). This unexpected concentration-dependent effect may be attributed to molecular aggregation at higher concentrations, which can reduce the number of freely diffusing monomeric molecules capable of efficiently interacting with bacterial membranes and intracellular targets. At the intermediate concentration (0.01 mg/mL), E5 molecules are more likely to remain monomeric, enhancing their penetration and binding to key bacterial components, thereby increasing antibacterial efficacy.

Table 3. Biological effectiveness of prepared compounds and control treatments (inhibition in cm)

Comp. No.	*E. coil*			*S. aureus*		
Conc. mg/ml	0.1	0.01	0.001	0.1	0.01	0.001
E_5	2.0	2.8	1.9	1.2	0.5	0.6
E_8	2.3	1.2	0.8	1.0	0.4	0.2
Ciprofloxacin	2.1	1.7	1.2	2.1	1.8	1.5
Amikacin	2.2	2.0	1.5	2.0	1.7	1.7

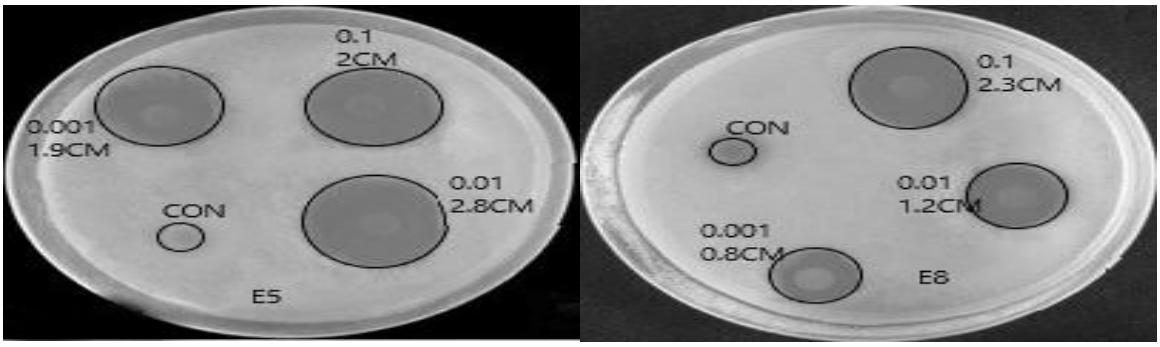


Fig. 5. The inhibition of compounds E5 and E8 against *E. coli.*

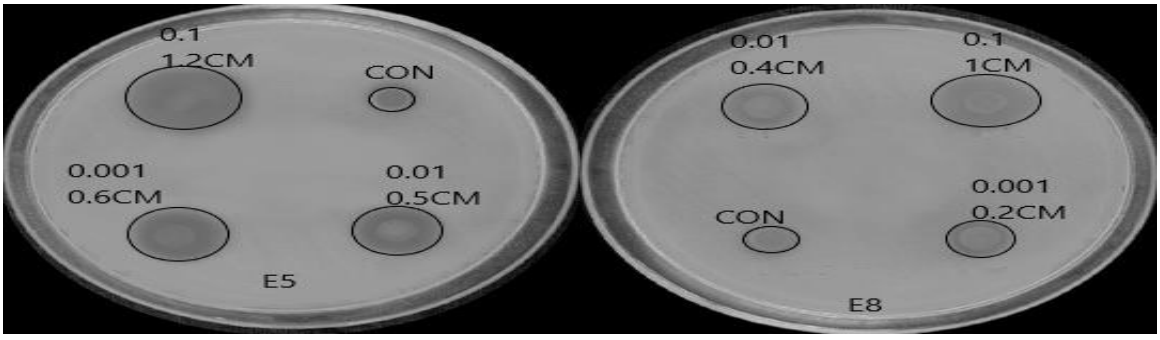


Fig. 6. The inhibition of compounds E5 and E8 against *Staph. aureus*.

The presence of bromine in E5 further contributes to its superior antibacterial activity. Halogen atoms are known to enhance lipophilicity, improve membrane permeability, and facilitate stronger interactions with bacterial biomolecules through halogen bonding or electrostatic interactions. In contrast, compound E8 contains a methyl group, which is smaller, nonpolar, and less capable of forming such interactions, resulting in comparatively lower activity and a strong dependence on concentration. Against *S. aureus*, both compounds displayed weaker activity than the reference

antibiotics, likely due to the thicker peptidoglycan layer in Gram-positive bacteria, which hinders compound diffusion (Fig. 6). Overall, these results indicate that E5, with its bromine substituent, is a promising antibacterial agent**,** particularly against Gram-negative strains, and highlight the significant role of halogen substitution in enhancing the activity of tetrazole derivatives [26–30].

3.4. Laser Activity Measurement Results for Some Prepared Compounds [31, 32]. Table 4 compares the effects of laser beams on the [E_5-E_8] compounds before and after irradiation, examining their color and melting points. All compounds are affected by irradiation, exhibiting a decrease in melting points. This confirms a decrease in thermal stability and an increase in molecular flexibility. Furthermore, the color changes reflect the presence of photochemicals or a change in electron levels. These compounds demonstrate their sensitivity to light and their susceptibility to structural modifications when exposed to irradiation.

Table 4. Results of exposing compounds [E_5-E_8] to laser Activity

Comp. No.	Before Irradiation		After Irradiation	
	M.P. ^{0}C	**Color**	**M.P. ^{0}C**	**Color**
E_5	263-265	Orange	251-252	Yellow
E_6	257-259	Brown	240-242	Light Brown
E_7	236-238	Light brown	221-223	Orange
E_8	244-246	White	232-235	Off-Whit

3.5. Molecular docking test results for a few produced chemicals [E_5, E_8]: [33, 34]. The enzyme biotin carboxylase (PDB:ID:3jzf) was selected for entry into the molecular docking system using the MOE 2014 program for compounds [E_5, E_8] that were found to have antibacterial activity against pathogenic *E. coli* bacteria. The derivative [E_5] exhibited a clear ability to disrupt the enzyme's binding site, as evidenced by a calculated anchoring value of -10.3 kcal/mol. Molecular conformation values (RMSD.i.b = 1.374 Å, RMSD.u.b = 2.237 Å) confirmed the accuracy and reliability of the binding process, with all values falling within the acceptable limit of less than 2.5 Å. The two-dimensional and three-dimensional analysis of the images revealed the formation of two hydrogen bonds between the amino acid residues Gly:B:114 and Gly:B:163 and the NH group on the tetrazole ring of the complex. Analyses also revealed a range of non-covalent interactions, including pi-anion, pi-cation, alkyl, pi-alkyl, pi-sigma, amide-pi stacked, and pi-alkyl, which contribute to the stability of the complex, as illustrated in Fig. 7.

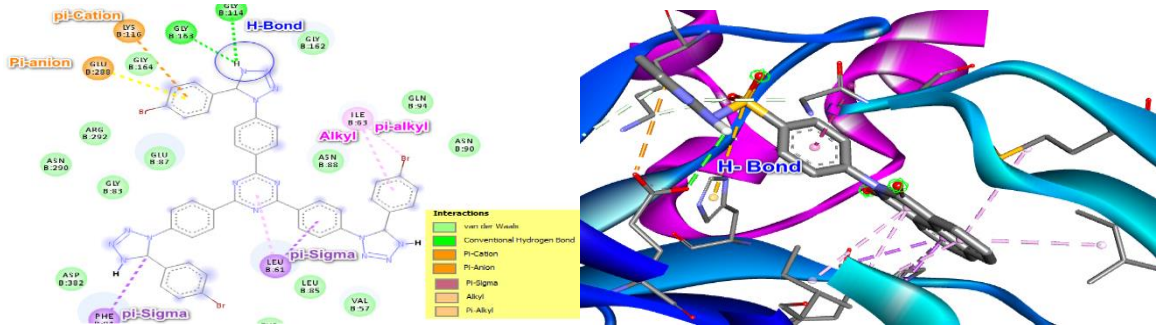


Fig. 7. 3D and 2D dimensions of compound [E_5]

Molecular docking results showed that compound [E_8] In the active site, it is bound at a degree of attachment -10.6 kcal/mol, and the corresponding values were found (RMSD.i.b = 4.979 Å, RMSD.u.b = 11.967 Å), indicating a greater difference in binding positions compared to other derivatives. Two-dimensional and three-dimensional images also revealed a hydrogen bond between the amino acid residue Gly:B:114 and the nitrogen atom in one of the tetrazole rings in the compound. Reaction analyses also revealed several types of non-covalent interactions, including pi-cation, alkyl, pi-alkyl, and pi-sigma interactions, suggesting that these interactions contribute to stabilizing the compound within the binding site, as illustrated in Fig. 8.

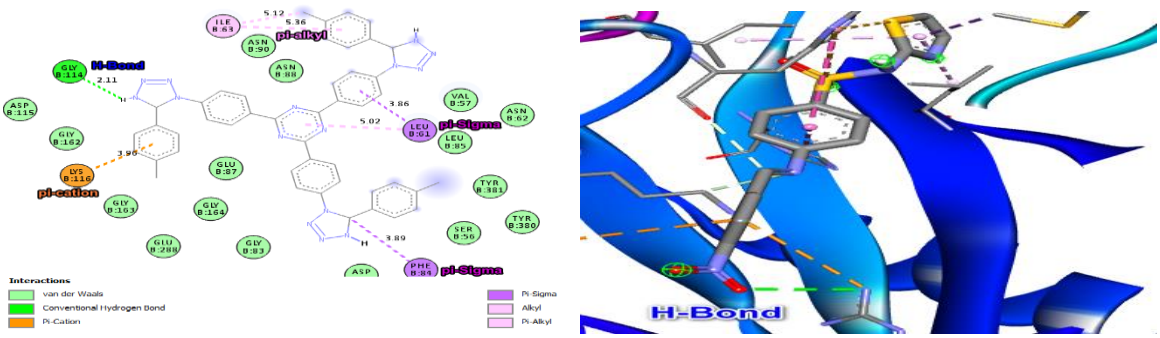


Fig. 8. 3D and 2D dimensions of compound [E_8]

Based on the previous molecular docking results, it can be concluded that derivative [E_5] is the most distinctive among the studied derivatives, exhibiting a lower interference energy value compared to compound [E_8], indicating a stronger binding affinity within the enzyme's binding site. [E_5] also showed favorable relative stability (RMSD) values, demonstrating good stability in the bound position. Although derivative [E_8] achieved a lower interference energy value, its relatively high RMSD values reduce the reliability of its positioning within the active site.

3.6. Study of liquid crystal phases: [35]. Studying liquid crystal phases using polarized light microscopy (POM) is a fundamental method for understanding the nature of phase transitions and the thermal behavior of anisotropic organic compounds (changes in physical properties). Therefore, in this work, compounds [E_5, E_8] were examined during heating and cooling to determine their liquid crystal phases, their thermal stability, and whether the identified crystalline phases were monophase or biphasic. POM images of compound [E_5] upon heating showed the presence of the hexagonal smectic phase (Colh), as shown in Fig. 9, followed by a transition to the nematic phase (N), as shown in Fig. 10. Thermal measurements showed that the Cr → Colh transition occurs at 255°C, while the Colh →N transition occurs at 272–290°C. This is attributed to the length of the terminal chain or the variation in side groups, in addition to the presence of several aromatic rings, which stabilize the molecule and increase its equatoriality, resulting in higher order and greater regularity.

As for the compound [E8], none of the liquid crystal phases appeared, as the reason is that the measurement does not range between 4.0 and 6.4 when measuring the ratio of the length of the molecule to its width.

Fig. 9. The fishy phase of [E_5] during heating

Fig. 10. The nematic phase of [E_5] during heating

Conclusions

The microwave-assisted synthesis of tetrazole derivatives proved to be efficient, rapid, and environmentally friendly, yielding well-characterized products as confirmed by FT-IR and 1H/13C-NMR spectra. Biological evaluation showed that E_5 exhibits superior antibacterial activity against *E. coli*, with the highest inhibition at 0.01 mg/mL. This is likely due to optimal monomeric

dispersion at this concentration, enhancing membrane penetration and intracellular interactions. The bromine atom in E_5 further enhances activity through increased lipophilicity and stronger interactions with bacterial targets. In contrast, E_8, containing a methyl group, showed activity mainly at the highest concentration, reflecting a strong concentration dependence. Both compounds were less effective against *S. aureus*, likely due to the thicker peptidoglycan layer of Gram-positive bacteria. Laser irradiation decreased melting points and changed colors, indicating structural sensitivity. Molecular docking confirmed that E_5 has the best binding and stabilization energy in biotin carboxylase, rationalizing its antibacterial superiority. Liquid crystal analysis revealed that E_5 exhibits clear smectic and nematic phases, whereas E_8 shows none, highlighting the role of structural features and halogen substitution in stabilizing mesophases. Overall, E_5 emerges as a promising multifunctional tetrazole derivative with potent antibacterial activity, laser responsiveness, effective molecular binding, and liquid crystalline behavior, making it a strong candidate for pharmaceutical applications.

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