PREPARATION AND CHARACTERIZATION OF SOME NEW TETRAZOLE DERIVATIVES AND MEASUREMENT OF THE BIOLOGICAL, LASER, AND COMPUTATIONAL ACTIVITY

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Abstract: *A series of novel tetrazole derivatives were successfully synthesized from Schiff bases and sodium azide using environmentally friendly methods. The structures of the compounds were confirmed through FT-IR, ^{1}H-NMR, and ^{13}C-NMR spectroscopy, verifying the formation of the tetrazole ring. The synthesized derivatives exhibited significant, concentration-dependent antibacterial activity against both Gram-positive (Staphylococcus aureus) and Gram-negative (Escherichia coli) strains, with variations in efficacy attributed to specific molecular substituents, highlighting clear structure–activity relationships. Laser irradiation studies using Nd:YAG laser beams revealed that the compounds maintain structural stability and physicochemical integrity under moderate exposure, while extended irradiation induced minor changes in melting points, R_f values, and color, indicating partial photochemical effects. Computational chemistry analyses, including total energy calculations, dipole moments, and HOMO–LUMO energy gaps, provided insight into the electronic properties, chemical reactivity, and stability of selected derivatives, with A_{18} predicted as the most reactive and A_{13} and A_{15} showing higher stability, correlating with observed biological activity. Overall, these findings demonstrate that the synthesized tetrazole derivatives are versatile compounds with promising applications in antibacterial therapy, laser-responsive processes, and molecular design, supporting their potential for further pharmaceutical and chemical investigations.*
Keywords*: tetrazole, Biological activity, laser effectiveness, Computational Chemistry.*

1. Introduction

Heterocyclic compounds have attracted considerable scientific interest in recent years due to their significant role in pharmacology and medicinal chemistry [1, 2]. Nitrogen-based heterocyclic molecules have attracted significant attention due to their extensive utility across industrial processes, synthetic organic methodologies, and pharmaceutical development [3]. Contemporary chemical research places a strong emphasis on designing synthetic strategies that are both sustainable and eco-conscious, aiming to reduce ecological impact without compromising reaction efficiency or product yield. Within the spectrum of heterocyclic frameworks, tetrazoles stand out as a notable category of five-membered rings, characterized by a structural arrangement of four nitrogen atoms and a single carbon atom, which imparts unique chemical and biological properties. Despite the continuous progress in heterocyclic chemistry, tetrazole derivatives continue to receive special attention because of their diverse applications in applied and medicinal chemistry. Tetrazole compounds were first synthesized in 1855, and since then, scientific publications related to these compounds and their practical applications have steadily increased [4]. Structurally, tetrazoles contain a high proportion of nitrogen–nitrogen and carbon–nitrogen bonds, which contributes to their thermal stability and often requires relatively high temperatures for their synthesis. Moreover, the relatively low carbon–hydrogen bond content in these molecules provides them with notable resistance to shock, electrostatic discharge, and other external stimuli [5]. These characteristics have made tetrazole derivatives important components in the development of many biologically active molecules capable of combating diseases caused by viruses and microorganisms [6]. Within the field of medicinal chemistry, tetrazole derivatives are commonly employed as bioisosteres for carboxylic acid moieties, offering a means to mimic the physicochemical and biological properties of these groups. Additionally, tetrazoles serve as versatile molecular linkers or spacers in drug design, facilitating the optimization of molecular geometry, receptor binding, and pharmacokinetic profiles [7].

Furthermore, tetrazole derivatives have been utilized in the design of energetic materials and serve as versatile building blocks for the synthesis of various heterocyclic systems. Tetrazole-containing frameworks have also been investigated as potential carriers in the design of anticancer agents, and several promising materials, including coordination compounds and natural products containing tetrazole moieties, have been reported [8].

Previous research has highlighted the significant antibacterial potential of tetrazole-containing compounds. Motivated by these findings, the current investigation focuses on the synthesis of a series of nitrogen-rich tetrazole derivatives utilizing alternative, eco-friendly methodologies. The target compounds were generated through the transformation of Schiff bases via reaction with sodium azide, resulting in the formation of five-membered tetrazole rings. This approach not only aligns with principles of green chemistry but also provides an efficient route for accessing structurally diverse tetrazole derivatives with potential biological activity. The biological activity of the synthesized compounds was evaluated against two types of bacteria, namely Gram-positive and Gram-negative strains. In addition, molecular docking studies were carried out for selected precursors and synthesized compounds to investigate their potential interactions with biological targets and to explore possible structure–activity relationships. Furthermore, the compounds were subjected to Nd:YAG laser irradiation to evaluate their photostability and potential laser-responsive properties, and computational chemistry analyses were performed to study electronic structures, HOMO–LUMO energies, and reactivity indices, providing insight into their chemical stability and potential activity [9].

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. Temperature measurements were performed using a 9300 electric thermocouple. Infrared spectra were recorded with a Shimadzu FT-IR 8400S spectrometer, employing potassium bromide (KBr) disks, over a spectral range of 400–4000 cm^{-1}. Proton (^{1}H) and carbon-13 (^{13}C) nuclear magnetic resonance (NMR) spectra were obtained using Bruker spectrometers operating at 400 MHz. Thin-layer chromatography (TLC) analyses were conducted on 0.2 mm thick silica gel plates activated with fluorescent silica gel G, with spots visualized under ultraviolet light. For microbiological experiments, the Advanced Microbiology Research Laboratory at Tikrit University sterilized culture media using a Rayba steam sterilizer (Spain). Petri dishes were subsequently incubated in a Heraeus D-63450 incubator (Germany) under controlled conditions.

2.3. Preparation of tetrazole derivatives [A_{13}-A_{18}] [10]. A quantity of 0.009 mol of the synthesized Schiff bases [A_1–A_6] was combined with 0.009 mol (0.6 g) of sodium azide dissolved in 15 mL of tetrahydrofuran (THF), while the Schiff bases were dissolved in 20 mL of the same solvent. The resulting mixture was stirred and maintained under reaction conditions for 8–9 hours, and the progression of the reaction was monitored and confirmed by thin-layer chromatography (TLC). Upon completion, the reaction mixture was allowed to cool to room temperature, followed by filtration and washing with cold water. The crude products were subsequently purified through recrystallization using tetrahydrofuran. Selected physical properties of the resulting tetrazole derivatives [A_{13}–A_{18}] are summarized in Table 1.

Table 1. Tetrazole derivatives' physical characteristics

Comp No.	R	Molecular Formula/	M.Wt g/mol	Color	Time (h)	M.P (^{0}C)	R*f*	Yield (%)
A_{13}	Br	$C_{14}H_{11}BrN_4O_2$	347.17	Light green	8	185-187	0.75	67
A_{14}	SCH_3	$C_{15}H_{14}N_4O_2S$	314.36	Dark yellow	8	171-173	0.66	71

A_{15}	OCH_3	$C_{15}H_{14}N_4O_3$	298.30	Light green	9	176-178	0.84	70
A_{16}	Cl	$C_{14}H_{11}ClN_4O_2$	302.72	Brown	9	187-190	0.73	64
A_{17}	$N(CH_3)_2$	$C_{16}H_{17}N_5O_2$	311.35	Green	9	149-151	0.61	61
A_{18}	CN	$C_{15}H_{11}N_5O_2$	293.29	Dark green	8	196-199	0.68	69

2.4. Biological activity study. In the Department of Biology laboratory, G-positive *S. aureus* and Gram-negative *E. coli* were the two kinds of bacteria that were identified. These are among the most common types of bacteria. Mueller-Hunter agar was prepared by dissolving 40 grams in 1 liter of distilled water and sterilizing it for 15 minutes at 1.5 bar. The solution was then poured into Petri dishes and allowed to cool [11-15]. Bacterial cells were placed on the dishes from three directions to ensure bacterial distribution. The synthesized compounds [A_{13}, A_{14}, A_{15}, A_{17}] were polarized and then diluted with dimethyl sulfoxide to several concentrations (0.1, 0.01, and 0.001 mg/mL). The dilution process began by dissolving 0.1 grams of the compounds in 10 mL of the solvent to obtain an initial dilution of 0.1 mg/mL. One milliliter of this dilution was transferred to another tube, and 9 milliliters of solvent were added [16, 17]. The solution was then diluted to produce a third dilution of 0.01 mg/mL. One milliliter of this dilution was then transferred to a new tube, and 9 milliliters of solvent were added to produce a third dilution of 0.001 mg/mL. Antibiotics such as ***amikacin and ciprofloxacin*** were used for comparison with the results of the prepared compounds. The plates were left to stand for 24 hours, and the results were read using a centimeter ruler [18, 19].

2.5. Testing the effectiveness of certain compounds against lasers. To expose the compounds [A_{13}, A_{14}, A_{15}, A_{16}, A_{17}, A_{18}] 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].

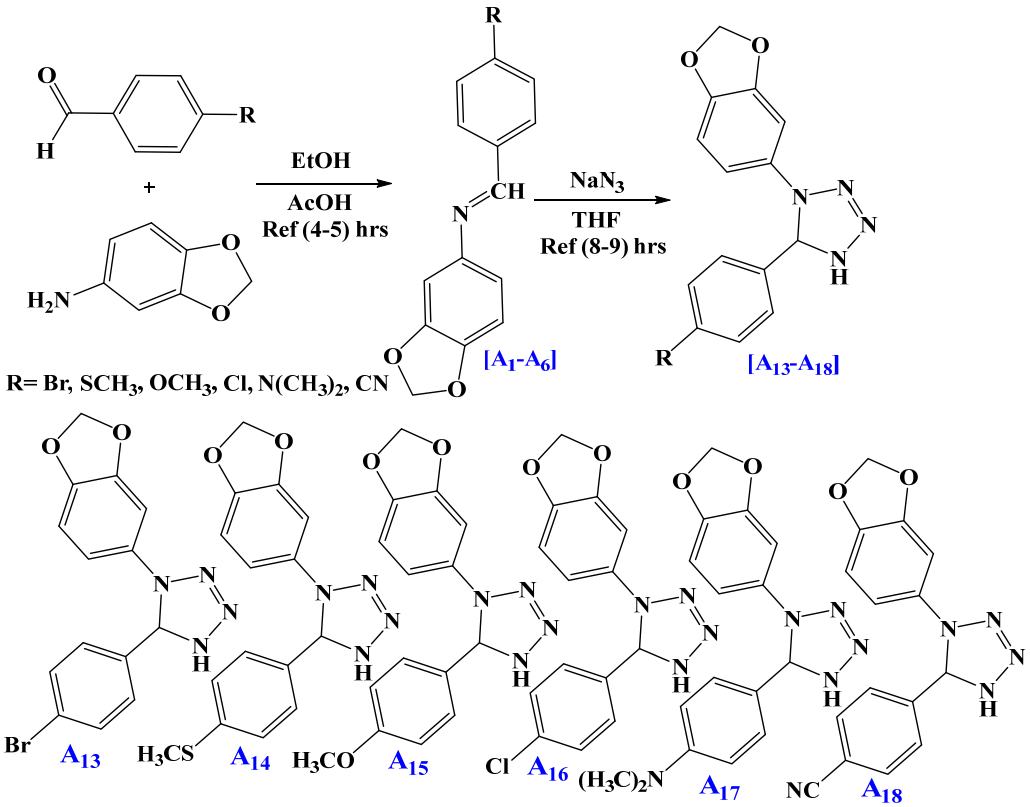
2.6. Theoretical Calculations for some compounds. Theoretical investigations of the synthesized compounds [A_{13}, A_{15}, A_{18}] were carried out using Gaussian 09W employing the AM1 semi-empirical approach. Initially, the molecular structures were sketched in two dimensions using ChemDraw within the ChemOffice suite and subsequently converted into three-dimensional representations using Chem3D. The resulting 3D geometries were refined with the Clean Up function, followed by energy minimization via the MM2 force field to determine the total energy of each molecule. Following geometry optimization, the energies of the frontier molecular orbitals—specifically the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO)—were calculated using Gaussian 09. The computationally derived molecular descriptors, including HOMO and LUMO energies, were exported and analyzed using Microsoft Excel to explore significant correlations between these electronic properties and other calculated physicochemical parameters.

3. Results and discussion

Our study aimed to form a number of new tetrazole compounds derived from Schiff bases prepared with sodium azide, as shown in Scheme 1.

3.1. Characterization of tetrazole derivatives [A_{13}-A_{18}]. FTIR analysis of the studied compounds [A_{13}-A_{18}] revealed the removal of the azomethine (C=N) band from the synthesized Schiff base [A_1-A_6], which is considered the core of the synthesis process. An extension band was found at (3240-3182) cm^{-1}, linked to (N-H) in tetrazole; an extension band at (3070-3041) cm^{-1}, linked to the aromatic (C-H) ligand; extension bands at (2972-2822) cm^{-1} and (2877-2852) cm^{-1}, linked to the aliphatic (CH) ligand; and two extension bands at (1587-1578) cm^{-1} and (1496-1465)

cm^{-1} associated with (C=C) in benzene. An elongation band at (1442-1417) cm^{-1} is associated with (N=N) within the formed tetrazole.



Scheme 1. Route of produced chemicals [A_7-A_{12}]

An elongation band at (1321-1306) cm^{-1} belonging to (C-O). An elongation band at (1234-1188) cm^{-1} belonging to (C-N) [23, 24] was also found, as shown in Table 2 and Fig.s 1 and 2.

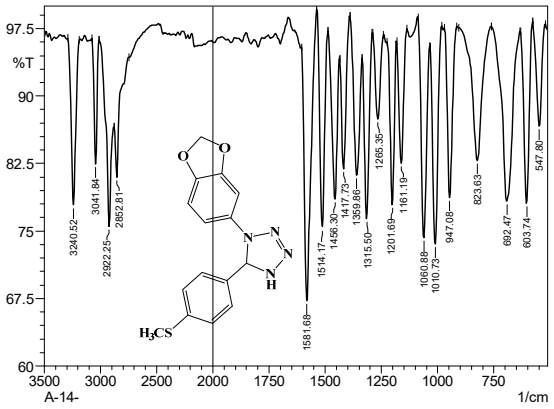


Fig. 1. FT-IR spectrum for A_{14} of

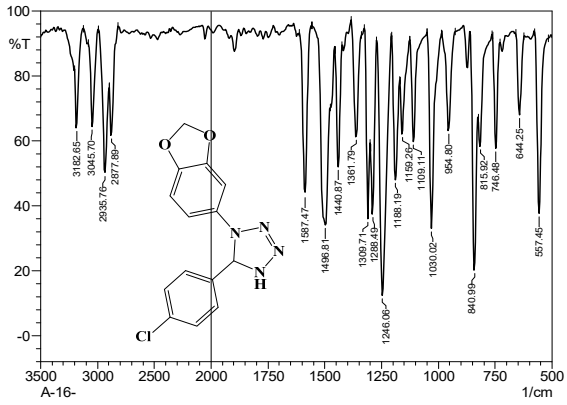


Fig. 2. FT-IR spectrum for A_{16}

When studying the ^{1}H-NMR nuclear magnetic resonance spectrum of compound [A_{15}] using the solvent (DMSO-d^6), a multiple signal appeared in the range (7.11-7.90) parts per million attributed to the protons of the aromatic rings; a single signal appeared at the chemical shift (5.90) parts per million attributed to the protons of the (CH_2) group; a single signal appeared at the chemical shift (5.21) parts per million attributed to the protons of the (CH) groups in the tetrazol ring; a single signal appeared at the chemical shift (3.73) parts per million attributed to the protons of the (O-CH_3) groups; a single signal appeared at the chemical shift (2.14) parts per million attributed to the protons of the (NH) groups, and a signal appeared at the chemical shift (2.52) parts per million attributed to the protons of the solvent (DMSO-d^6), as in Fig. 3.

Table 2. Tetrazole derivative FT-IR absorption data

Comp. No.	R	IR (KBr) cm-1							
		ν N-H	ν C-H Arom.	νC-H *asy. sym.*	ν C=C Arom.	ν N=N	ν C-O	ν C-N	Others
A_{13}	Br	3231	3051	2943 / 2865	1584 / 1471	1432	1313	1209	ν C-Br 533
A_{14}	SCH_3	3240	3041	2922 / 2852	1581 / 1456	1417	1315	1201	ν C-S 947
A_{15}	OCH_3	3216	3066	2971 / 2885	1578 / 1464	1425	1321	1234	---
A_{16}	Cl	3182	3045	2935 / 2877	1587 / 1496	1440	1309	1188	ν C-Cl 746
A_{17}	$N(CH_3)_2$	3198	3070	2960 / 2855	1586 / 1482	1442	1321	1212	---
A_{18}	CN	3223	3059	2972 / 2868	1583 / 1489	1438	1306	1231	ν C≡N 2208

When the ^{13}C-NMR spectrum of compound [A_{15}] was studied using the solvent (DMSO-d^6), multiple signals were observed at chemical shifts (154.27, 142.10, 140.30, 139.08, 134.41, 132.65, 131.80, 129.52, 127.13, 123.66) ppm, attributed to the aromatic ring carbons; a signal at chemical shift (102.44) ppm, attributed to the (2CH) group; a signal at chemical shift (92.22) ppm, attributed to the (CH) group in the tetrazol ring; a signal at chemical shift (56.52) ppm, attributed to the (O-CH3) group; and a signal at chemical shift (39.37-40.62) ppm. The million is attributed to the solvent carbon (DMSO-d^6), and the spectrum is shown in Fig. 4.

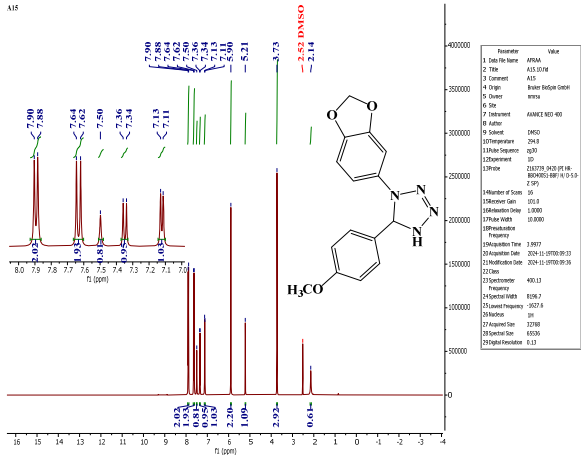


Fig. 3. ^{1}H-NMRspectrum for A_{15}

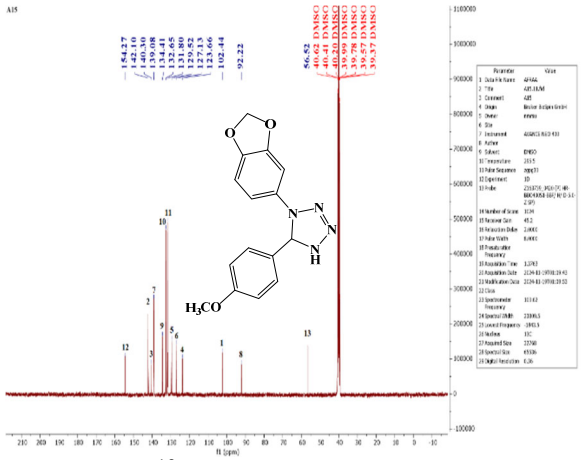


Fig. 4. ^{13}C-NMR spectrum for A_{15}

3.2. Assessment of Prepared Compounds' Biological Activity. The synthesized tetrazole derivatives were evaluated for their antibacterial activity against *Escherichia coli* and *Staphylococcus aureus* at concentrations of 0.1, 0.01, and 0.001 mg/mL, with *Ciprofloxacin* and *Amikacin* as references. As shown in Table 3, all compounds exhibited concentration-dependent activity, with inhibition zones decreasing at lower concentrations.

Table 3. Inhibition values in centimeters for some synthetic compounds

Comp. No.	*E. coil*			*S. aureus*		
Conc. mg/ml	0.1	0.01	0.001	0.1	0.01	0.001
A_{13}	2.3	2.2	1.9	1.9	1.8	1.7
A_{14}	2.0	1.8	1.7	2.4	2.2	2.2
A_{15}	2.1	1.9	1.5	1.7	1.5	1.3
A_{17}	2.3	1.9	1.7	1.5	1.3	1.3

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

Against *E. coli*, compounds A_{13} and A_{17} showed the highest activity (2.3 cm at 0.1 mg/mL), comparable to or slightly exceeding the reference antibiotics, while A_{14} and A_{15} displayed moderate effects (Fig. 5). For *S. aureus*, A_{14} demonstrated the strongest inhibition (2.4 cm at 0.1 mg/mL), surpassing the standards, whereas the other compounds exhibited moderate activity (Fig. 6). These results indicate that the tetrazole derivatives possess notable antibacterial potential, with their activity influenced by structural features and substituents, suggesting their suitability as candidates for further antimicrobial development [25-29].

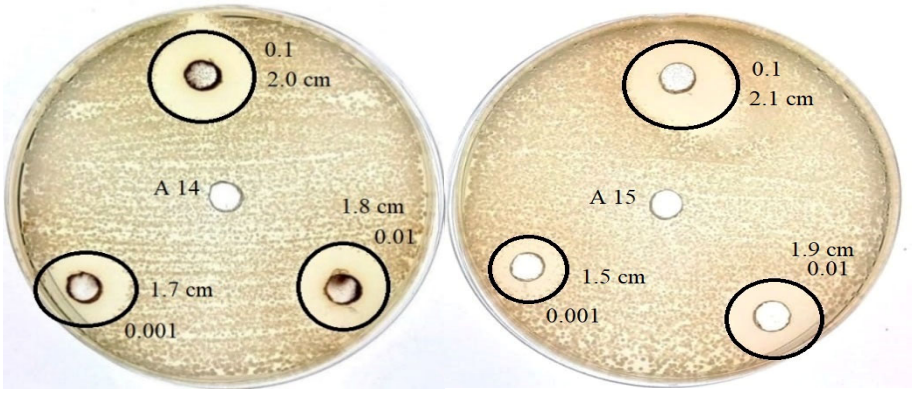


Fig. 5. The inhibition of compounds A_{14} and A_{15} against *E. coli.*

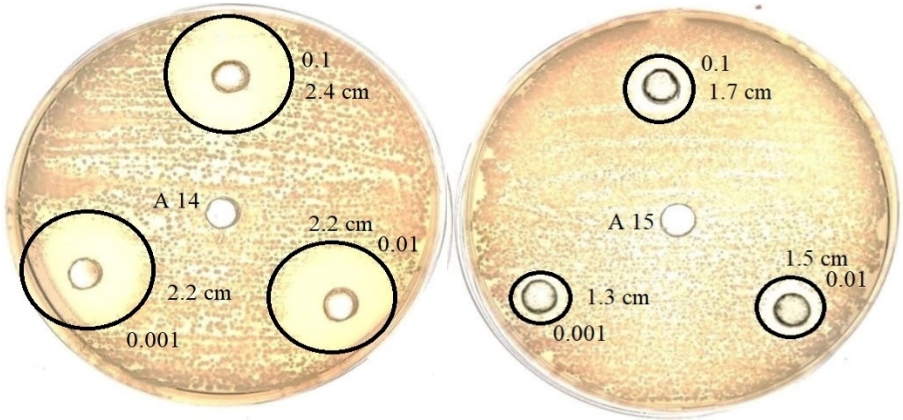


Fig. 6. The inhibition of compounds A_{14} and A_{15} against *Staph. aureus*.

3.3. Laser Activity Measurement Results for Some Prepared Compounds [30]. The results presented in Table 4 illustrate the effect of laser irradiation time (15, 30, 45, and 60 seconds) on the physical properties of the synthesized compounds A_{13}, A_{16}, and A_{17}. As shown in the table, the compounds exposed to laser irradiation for 15–45 seconds exhibit very similar physicochemical characteristics, including nearly identical Rf values, melting points, and colors, indicating that moderate laser exposure does not significantly affect the structural stability or purity of the compounds. For example, compound A_{13} shows an Rf value of 0.75 and a melting point of 185–187 °C with a light green color for irradiation times between 15 and 45 seconds, whereas after 60 seconds of irradiation the Rf value decreases slightly to 0.69, the melting point shifts to 172–174 °C, and the color changes to light yellow. A comparable pattern is observed for compounds A_{16} and A_{17}, where extended irradiation at 60 seconds leads to slight reductions in Rf values and melting points along with noticeable color changes. These observations suggest that prolonged laser exposure may induce minor modifications in the compounds, possibly due to partial photochemical effects or slight

degradation. Overall, the data reported in Table 4 indicate that shorter irradiation times preserve the stability and purity of the synthesized compounds, while longer exposure times may lead to detectable variations in their physical properties.

Table 4. Results of exposing compounds [A_{13}, A_{16}, A_{17}] to laser activity

Comp No.	15 S			30 S			45 S			60 S		
	Color	**M.P (^{0}C)**	**R*f***	**Color**	**M.P (^{0}C)**	**R*f***	**Color**	**M.P (^{0}C)**	**R*f***	**Color**	**M.P (^{0}C)**	**R*f***
A_{13}	Light green	185-187	0.75	Light green	185-187	0.75	Light green	185-187	0.75	Light Yello	172-174	0.69
A_{16}	Brown	187-190	0.73	Brown	187-190	0.73	Brown	187-190	0.73	Light Brown	167-169	0.60
A_{17}	Green	149-152	0.61	Green	149-152	0.61	Green	149-152	0.61	Light Green	136-138	0.55

3.4. Computational Chemistry of compounds [A_{13}, A_{15}, A_{18}] [31]. The computational chemistry results for compounds A_{13}, A_{15}, and A_{18} provide insight into their electronic properties, stability, and potential reactivity. As shown in the table, the total energies of the molecules range from 14.65 to 20.02 kJ, with A_{15} exhibiting the highest total energy (20.0171 kJ), suggesting slightly lower thermodynamic stability compared to A_{13} and A_{18}. The dipole moments (μ) vary from 0.0383 to 0.0250 Debye, with A_{18} having the lowest value, indicating a more symmetric charge distribution and potentially lower polarity. The calculated HOMO and LUMO energies reveal that the energy gaps (EHOMO–ELUMO) range from 0.0500 to 0.0786 kcal/mol, with A_{18} showing the smallest gap, implying higher chemical reactivity and increased potential for electron transfer interactions. The electrophilicity index (ω) and chemical potential (μ) further support these observations, suggesting that A_{18} could be more reactive toward nucleophilic species, while A_{13} and A_{15} are relatively more stable. Overall, these computational results indicate that subtle differences in electronic properties among the tetrazole derivatives can influence their chemical stability and reactivity, which may correlate with their biological activity and interactions in molecular docking studies (Table 5).

Table 5. Calculated values for some computational properties of the prepared compounds

No	Property (Kcal)								Dipole moment (Debye)	Energy Kj
	E_{LUMO}	**E_{HOMO}**	**E_{HOMO} -E_{LUMO}**	***I***	***A***	**μ**	**η**	**ω**		
A_{13}	-0.16929	-0.24605	-0.0767	0.24605	0.16929	0.2076	0.0383	2.82673 E-05	0.6624	14.6506
A_{15}	-0.16740	-0.24600	-0.0786	0.24600	0.16740	0.2067	0.0393	3.03492 E-05	0.6212	20.0171
A_{18}	-0.19605	-0.24606	-0.0500	0.24606	0.19605	0.2210	0.0250	7.81719 E-06	0.6824	14.7327

Conclusions

The present study demonstrates that a series of novel tetrazole derivatives were successfully synthesized from Schiff bases and sodium azide using environmentally friendly methods, with their structures confirmed by FT-IR, ^{1}H-NMR, and ^{13}C-NMR analyses. The compounds exhibited significant, concentration-dependent antibacterial activity against both *Staphylococcus aureus* and *Escherichia coli*, with variations in efficacy linked to molecular substituents, highlighting clear structure–activity relationships. Exposure to Nd:YAG laser irradiation showed that these derivatives maintain stability under laser conditions, suggesting potential applications in photochemical and laser-assisted processes. Computational analyses further revealed that electronic properties, including HOMO–LUMO gaps, dipole moments, and electrophilicity indices, influence molecular reactivity

and stability, with compound A_{18} predicted to be the most reactive, while A_{13} and A_{15} are comparatively more stable, correlating with their observed biological behavior. Collectively, these findings indicate that the synthesized tetrazole derivatives are versatile compounds with promising applications in antibacterial therapy, photochemistry, and molecular design, supporting their potential for further pharmaceutical and chemical investigations.

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