SYNTHESIS, SPECTROSCOPIC CHARACTERIZATION AND IN VITRO DNA INTERACTION STUDIES OF POLY(1,2,4-TRIAZOLYL) BORATE COMPLEXES CONTAINING BIOLOGICALLY RELEVANT METAL IONS: A SECONDARY DATA-BASED REVIEW AND COMPARATIVE ANALYSIS

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Abstract

Poly(1,2,4-triazolyl) borate ligands have attracted considerable attention in coordination chemistry because of their versatile coordination behavior, structural stability, and potential biological applications. This study presents a secondary data-based review of the synthesis, spectroscopic characterization, and *in vitro* DNA interaction studies of poly(1,2,4-triazolyl) borate complexes containing biologically relevant metal ions reported in the scientific literature before 2025. Published research was systematically examined to compare synthetic approaches, coordination modes, and characterization techniques, including Fourier-transform infrared (FTIR), ultraviolet-visible (UV–Vis), nuclear magnetic resonance (NMR), mass spectroscopy, and elemental analysis. The reviewed studies indicate that metal coordination significantly influences the physicochemical properties, stability, and DNA-binding behavior of these complexes through intercalative, groove-binding, or electrostatic interactions. Comparative analysis demonstrates that spectroscopic characterization provides reliable evidence for complex formation and supports the interpretation of biological activity. The findings consolidate existing knowledge, identify prevailing research trends and gaps, and provide a comprehensive reference for future investigations aimed at developing poly(1,2,4-triazolyl) borate metal complexes with enhanced bioinorganic and medicinal applications.

Keywords: Poly(1,2,4-triazolyl) borate, coordination chemistry, biologically relevant metal ions, spectroscopic characterization, DNA interaction, secondary data analysis, bioinorganic chemistry.

2. Introduction

2.1 Background

Coordination chemistry has emerged as one of the most dynamic branches of inorganic chemistry due to its significant contributions to catalysis, materials science, environmental chemistry, and medicinal applications. The formation of coordination compounds through the interaction of metal ions with electron-donating ligands has enabled the development of molecules possessing unique structural, electronic, and biological properties. The coordination environment surrounding a metal center plays a crucial role in determining the physicochemical characteristics, stability, and reactivity of the resulting complexes. Consequently, the rational design of ligands capable of forming stable and versatile coordination frameworks has become an important area of contemporary chemical research (Cotton et al., 1999; Housecroft& Sharpe, 2018).

Among the numerous classes of nitrogen-containing ligands, triazole-based ligands have attracted considerable scientific interest because of their strong coordinating ability, electronic versatility, and capacity to stabilize metal ions in different oxidation states. The presence of multiple nitrogen donor atoms within the triazole ring facilitates diverse coordination

modes, allowing the formation of mono-, bi-, and polynuclear metal complexes with well-defined geometries. These structural characteristics have encouraged extensive investigations into their applications in bioinorganic chemistry, supramolecular chemistry, molecular recognition, and medicinal chemistry (Haasnoot, 2000).

Borate-based ligands represent another important family of ligands in coordination chemistry owing to their remarkable structural flexibility and ability to support multidentate coordination. Polyborate ligands provide robust frameworks that enhance the stability of transition metal complexes while permitting structural modifications through ligand functionalization. The incorporation of heterocyclic nitrogen donors such as 1,2,4-triazole into borate frameworks further improves coordination efficiency by combining the electronic properties of triazole rings with the structural stability imparted by borate moieties. Such hybrid ligand systems exhibit excellent chelating capabilities and have become increasingly relevant in the design of functional coordination compounds.

Poly(1,2,4-triazolyl) borate ligands constitute a distinctive class of scorpionate-type ligands that coordinate to metal ions through multiple nitrogen donor atoms while maintaining a stable borate backbone. Their versatile coordination behavior enables the formation of complexes with various biologically relevant transition metals, producing compounds with diverse geometrical arrangements and physicochemical properties. The adaptability of these ligands allows modulation of metal–ligand interactions, thereby influencing molecular stability, electronic configuration, and biological activity. These characteristics have stimulated growing interest in exploring their synthesis and structural characterization using advanced analytical techniques.

In recent years, research involving poly(1,2,4-triazolyl) borate metal complexes has expanded beyond structural chemistry toward biological investigations. Spectroscopic characterization techniques, including Fourier-transform infrared spectroscopy (FTIR), ultraviolet–visible (UV–Vis) spectroscopy, nuclear magnetic resonance (NMR), mass spectrometry, elemental analysis, and magnetic susceptibility measurements, are routinely employed to establish coordination modes and confirm complex formation. Furthermore, the increasing recognition of metal-based compounds as potential therapeutic agents has prompted extensive investigations into their interactions with biomolecules, particularly deoxyribonucleic acid (DNA), which serves as a primary molecular target in many biological and pharmacological processes.

Because numerous experimental studies published before 2025 have independently reported the synthesis, characterization, and biological evaluation of triazole-derived metal complexes, a comprehensive secondary-data-based assessment is valuable for consolidating existing knowledge. Such an approach facilitates comparison of synthetic methodologies, coordination behavior, spectroscopic characteristics, and reported biological interactions, thereby providing a broader understanding of the scientific progress achieved in this field and identifying directions for future research.

2.2 Importance of Biologically Relevant Metal Ions

Biologically relevant transition metal ions play a fundamental role in coordination chemistry and bioinorganic research because of their diverse oxidation states, variable coordination geometries, and ability to participate in essential biological processes. The incorporation of metal ions into ligand frameworks often modifies the electronic structure, stability, reactivity, and biological activity of coordination compounds. Consequently, transition metal complexes have attracted considerable attention as potential antimicrobial, antioxidant, anticancer, and DNA-binding agents. The selection of an appropriate metal ion is therefore a critical factor influencing the structural and functional properties of poly(1,2,4-triazolyl) borate complexes (Housecroft& Sharpe, 2018; Bertini et al., 2007).

Among the biologically important transition metals, cobalt(II) [Co(II)] is widely recognized for its flexible coordination behavior and ability to adopt tetrahedral or octahedral geometries

depending on the ligand environment. Cobalt complexes exhibit favorable redox properties and have been investigated for their catalytic activity, enzyme mimicking behavior, antimicrobial potential, and interactions with nucleic acids. Coordination with poly(1,2,4-triazolyl) borate ligands enhances the structural stability of Co(II) complexes while providing opportunities to investigate their physicochemical and biological characteristics.

Nickel(II) [Ni(II)] is another biologically relevant metal ion that forms stable complexes with nitrogen-donor ligands. Owing to its preference for octahedral and square-planar coordination geometries, Ni(II) serves as an excellent model for studying metal–ligand interactions and electronic structures. Nickel-containing coordination compounds have demonstrated promising catalytic, antimicrobial, and DNA-binding properties. The strong affinity of Ni(II) toward triazole nitrogen atoms facilitates the formation of well-defined coordination frameworks suitable for spectroscopic and structural investigations (Cotton et al., 1999).

Copper(II) [Cu(II)] occupies a prominent position in medicinal inorganic chemistry because of its redox activity and indispensable biological functions. As a constituent of numerous metalloenzymes involved in electron transport, oxidative stress regulation, and cellular respiration, copper is essential for normal physiological processes. Copper(II) complexes frequently display enhanced biological activity compared with their corresponding free ligands, particularly in DNA-binding and DNA-cleavage studies. Their variable coordination geometries and favorable electronic characteristics make Cu(II)-based poly(1,2,4-triazolyl) borate complexes attractive candidates for investigating structure–activity relationships (Lippard & Berg, 1994).

Zinc(II) [Zn(II)] differs from many transition metals because of its filled d^{10} configuration, which renders it redox-inactive under physiological conditions. Despite the absence of redox activity, zinc performs indispensable structural and catalytic functions in numerous enzymes and transcription factors. Zinc complexes are generally characterized by low toxicity, high kinetic stability, and strong affinity for nitrogen-containing ligands. These properties make Zn(II) an important metal ion for evaluating coordination behavior and biomolecular interactions without complications arising from redox reactions. Zinc complexes have therefore received considerable attention in studies involving DNA binding, enzyme inhibition, and pharmaceutical applications.

Manganese(II) [Mn(II)] is another essential trace metal involved in several biological processes, including antioxidant defense, photosynthesis, and enzymatic catalysis. Manganese-containing enzymes play crucial roles in protecting cells against oxidative damage through the activity of manganese superoxide dismutase. Mn(II) complexes exhibit diverse coordination geometries and have been explored for their catalytic efficiency, antioxidant properties, and interactions with biomolecules. Coordination with poly(1,2,4-triazolyl) borate ligands may improve the stability and biological performance of Mn(II) complexes, thereby broadening their potential applications in bioinorganic chemistry.

Collectively, Co(II), Ni(II), Cu(II), Zn(II), and Mn(II) provide an excellent platform for investigating the influence of metal-ion characteristics on the synthesis, coordination behavior, spectroscopic properties, and biological activities of poly(1,2,4-triazolyl) borate complexes. Comparative evaluation of these metal ions using secondary data from published studies enables a deeper understanding of how variations in ionic radius, electronic configuration, coordination preference, and redox behavior affect complex stability and *in vitro* DNA interaction. Such knowledge is valuable for the rational design of novel metal-based compounds with improved structural characteristics and potential biomedical applications.

2.3 Importance of Spectroscopic Characterization

Spectroscopic characterization is a fundamental component of coordination chemistry, providing reliable evidence for the synthesis, composition, and structural features of metal complexes. The combined application of complementary analytical techniques enables accurate

determination of coordination modes, bonding interactions, electronic environments, and molecular geometry. In studies involving poly(1,2,4-triazolyl) borate complexes, spectroscopic analyses are essential for confirming successful ligand coordination and evaluating the influence of different metal ions on the structural and physicochemical properties of the resulting complexes (Nakamoto, 2009; Lever, 1984).

Fourier-transform infrared (FTIR) spectroscopy is widely employed to identify characteristic functional groups and monitor shifts in vibrational frequencies associated with metal–ligand bond formation. Ultraviolet–visible (UV–Vis) spectroscopy provides valuable information regarding electronic transitions, ligand-field effects, and coordination geometry. Nuclear magnetic resonance (NMR) spectroscopy, particularly for diamagnetic complexes, offers detailed insights into the chemical environment of ligand nuclei and confirms structural integrity. Mass spectrometry facilitates molecular weight determination and verifies the molecular composition of synthesized complexes, while elemental analysis establishes the empirical formula and purity of the compounds. Additionally, magnetic susceptibility measurements assist in determining the oxidation state, spin configuration, and coordination geometry of transition metal ions.

The integration of these characterization techniques provides a comprehensive understanding of the structural and electronic properties of poly(1,2,4-triazolyl) borate complexes. Such information forms the basis for correlating molecular structure with biological activity, particularly in *in vitro* DNA interaction studies and other bioinorganic applications.

2.4 Importance of DNA Interaction Studies

The investigation of DNA interactions has become a central aspect of bioinorganic and medicinal chemistry because deoxyribonucleic acid (DNA) serves as the primary repository of genetic information and a major molecular target for numerous therapeutic agents. Metal complexes capable of interacting with DNA have attracted considerable interest owing to their potential applications in antimicrobial, anticancer, and antiviral drug development. The nature and strength of DNA binding are largely influenced by the coordination environment of the metal center, ligand architecture, and physicochemical properties of the complex (Lippard & Berg, 1994; Sigel & Sigel, 1996).

Poly(1,2,4-triazolyl) borate metal complexes can interact with DNA through several binding mechanisms, including **intercalation**, **groove binding**, and **electrostatic interactions**. Intercalation involves the insertion of planar aromatic ligand moieties between adjacent DNA base pairs, resulting in enhanced complex stability and alterations in DNA conformation. Groove binding occurs when the complex associates with the major or minor groove of the DNA double helix through hydrogen bonding and van der Waals interactions, whereas electrostatic interactions arise from the attraction between positively charged metal complexes and the negatively charged phosphate backbone of DNA. These distinct binding modes influence the biological activity and therapeutic potential of coordination compounds.

Evaluation of *in vitro* DNA interactions using spectroscopic and biophysical techniques provides valuable insights into the binding affinity, mode of interaction, and structural effects of metal complexes on DNA. Such studies contribute significantly to understanding structure–activity relationships and support the rational design of novel poly(1,2,4-triazolyl) borate complexes with improved biomedical and pharmaceutical applications.

2.5 Research Gap

Although numerous studies published before 2025 have reported the synthesis and characterization of triazole-derived metal complexes, the available literature remains largely fragmented, with most investigations focusing on individual ligands or specific transition metal ions. Comparative analyses integrating the synthesis, spectroscopic characterization, and *in vitro* DNA interaction behavior of poly(1,2,4-triazolyl) borate complexes containing biologically relevant metal ions are relatively limited. Furthermore, variations in experimental methodologies and

characterization approaches have hindered comprehensive evaluation of structure–property relationships. Therefore, a systematic secondary-data-based assessment is required to consolidate existing findings, identify common trends, compare coordination behavior, and highlight future research opportunities in this important area of coordination and bioinorganic chemistry.

2.6 Objectives

The present study was undertaken with the following objectives:

1. To review the reported synthesis strategies of poly(1,2,4-triazolyl) borate complexes containing biologically relevant metal ions using published secondary data.
2. To compare the spectroscopic characterization of the synthesized metal complexes based on FTIR, UV–Visible spectroscopy, NMR, mass spectrometry, elemental analysis, and magnetic susceptibility studies.
3. To evaluate the coordination behavior and structural characteristics of Co(II), Ni(II), Cu(II), Zn(II), and Mn(II) complexes reported in the literature.
4. To analyze and compare the *in vitro* DNA-binding characteristics and interaction mechanisms of the reported metal complexes.
5. To identify current research trends, existing knowledge gaps, and future directions for the development of poly(1,2,4-triazolyl) borate-based coordination compounds with potential bioinorganic and medicinal applications.

3.1 Theoretical Background: Development of Poly(1,2,4-Triazolyl) Borate Ligands

Poly(1,2,4-triazolyl) borate ligands belong to a broader class of nitrogen-rich borate ligands that have become important in coordination chemistry because they can bind metal ions through multiple donor atoms while providing a stable borate framework. The combination of a borate center with 1,2,4-triazole rings produces ligands that are electronically versatile and capable of forming stable coordination complexes with transition metals.

The concept of borate-based ligands originated from the development of scorpionate ligands, in which a boron atom serves as a central anchoring unit attached to several nitrogen-containing heterocyclic rings. This structural arrangement allows the ligand to coordinate to a metal center through multiple nitrogen donor atoms, producing chelate rings that enhance complex stability. Compared with simple monodentate ligands, poly(1,2,4-triazolyl) borate ligands generally exhibit greater kinetic and thermodynamic stability because of the chelate effect.

The **1,**2,4-triazole ring is particularly attractive as a donor group because it contains three nitrogen atoms capable of participating in coordination. Depending on the position of coordination and the electronic properties of the metal ion, triazole ligands may act as monodentate, bidentate, or bridging ligands. This versatility enables the formation of coordination compounds with diverse geometries, including tetrahedral, square-planar, trigonal bipyramidal, and octahedral structures. The ability to adopt different coordination modes makes poly(1,2,4-triazolyl) borate ligands valuable building blocks for designing new metal complexes.

From an electronic perspective, the borate moiety provides structural rigidity while the triazole rings contribute electron density to the coordinated metal ion through σ-donation and, in some cases, π-interactions. The balance between these electronic effects influences the stability, geometry, magnetic properties, and reactivity of the resulting complexes. Consequently, subtle modifications in ligand structure or substitution pattern can significantly alter the physicochemical characteristics of the coordinated metal species.

Theoretical principles of coordination chemistry also suggest that the properties of poly(1,2,4-triazolyl) borate complexes depend strongly on the electronic configuration of the coordinated metal ion. Transition metals possessing partially filled d-orbitals interact differently with nitrogen donor ligands according to crystal field theory and ligand field theory. These interactions determine ligand-field stabilization energy, preferred coordination geometry,

magnetic behavior, and spectroscopic characteristics. Therefore, identical ligands may produce structurally distinct complexes when coordinated with different metal ions such as Co(II), Ni(II), Cu(II), Zn(II), or Mn(II).

Another important theoretical aspect is the relationship between ligand architecture and biological activity. Nitrogen-containing heterocyclic ligands are frequently associated with enhanced biological properties because they improve metal ion stabilization under physiological conditions and facilitate interactions with biomolecules. Poly(1,2,4-triazolyl) borate complexes often possess suitable electronic distribution and molecular stability for interacting with nucleic acids and proteins. Their coordination environment can influence DNA-binding affinity, cellular uptake, and overall biological performance, making them promising candidates in bioinorganic and medicinal chemistry.

3.2 Theoretical Perspectives on the Synthesis of Transition Metal Complexes

The synthesis of transition metal complexes is a fundamental aspect of coordination chemistry that involves the interaction of metal ions with ligands containing suitable electron-donating atoms. The formation of coordination compounds is governed by the Lewis acid–base concept, where transition metal ions function as Lewis acids by accepting electron pairs from donor ligands acting as Lewis bases. The stability and properties of the resulting complexes depend on several factors, including the electronic configuration of the metal ion, ligand denticity, reaction conditions, and thermodynamic stability.

Poly(1,2,4-triazolyl) borate ligands are particularly suitable for transition metal coordination because they contain multiple nitrogen donor atoms capable of forming coordinate covalent bonds with metal centers. The borate framework acts as a stable scaffold, while the triazole rings provide flexible coordination sites that facilitate the formation of mono-, bi-, or polynuclear complexes. Theoretical principles of chelation indicate that multidentate ligands generally produce more stable complexes than monodentate ligands due to the chelate effect, which enhances both kinetic and thermodynamic stability.

The selection of transition metal ions plays a decisive role in determining the structure and properties of the synthesized complexes. Biologically relevant metal ions such as cobalt(II), nickel(II), copper(II), zinc(II), and manganese(II) exhibit distinct electronic configurations and coordination preferences. Consequently, the same ligand may generate coordination compounds with different geometries, coordination numbers, magnetic properties, and biological activities. Crystal field theory and ligand field theory explain these variations by describing the interaction between the metal d-orbitals and the ligand donor atoms, which influences electronic transitions, orbital splitting, and overall complex stability.

The synthesis of poly(1,2,4-triazolyl) borate metal complexes generally involves the reaction of the ligand with an appropriate metal salt under controlled experimental conditions. Parameters such as solvent polarity, pH, temperature, reaction time, and metal-to-ligand molar ratio significantly influence the coordination process and the purity of the final product. Polar solvents are commonly preferred because they facilitate dissolution of both the ligand and metal salts, thereby promoting efficient coordination. Similarly, maintaining an appropriate pH prevents unwanted hydrolysis or precipitation of metal hydroxides, ensuring the successful formation of coordination complexes.

Reaction temperature also plays a critical role during synthesis. Moderate heating often accelerates coordination reactions by increasing molecular collisions and enhancing reaction kinetics, whereas excessively high temperatures may lead to ligand decomposition or undesirable side reactions. Likewise, sufficient reaction time is required to achieve equilibrium and maximize complex yield. Optimization of these experimental variables is therefore essential for obtaining pure and structurally well-defined coordination compounds.

Following complex formation, purification procedures such as filtration, recrystallization,

washing with suitable solvents, and vacuum drying are employed to remove unreacted starting materials and impurities. The purity of the isolated complexes is essential because contaminants may interfere with subsequent spectroscopic characterization and biological evaluation. Theoretical considerations suggest that highly pure coordination compounds provide more reliable structural and physicochemical data, thereby improving the interpretation of experimental results.

Another important theoretical aspect of synthesis is the relationship between molecular structure and functional performance. The geometry adopted by the metal center directly influences the electronic distribution, coordination stability, and accessibility of reactive sites within the complex. These structural features subsequently affect interactions with biological macromolecules, including DNA and proteins. Therefore, rational synthesis aims not only to obtain stable coordination compounds but also to tailor their physicochemical properties for specific biological or catalytic applications.

3.3 Theoretical Aspects of Spectroscopic Characterization

Spectroscopic characterization is an indispensable component of coordination chemistry because it provides experimental evidence for the formation, composition, and structural features of metal complexes. Since no single analytical technique can completely describe a coordination compound, researchers employ multiple complementary methods to obtain comprehensive information regarding molecular structure, bonding, and electronic properties.

Fourier-transform infrared (FTIR) spectroscopy is commonly used to identify functional groups and investigate metal–ligand coordination. Coordination typically alters the vibrational frequencies of donor groups, allowing researchers to infer the participation of nitrogen-containing triazole rings in bond formation with the metal center. FTIR therefore serves as an important qualitative tool for confirming successful complexation.

Ultraviolet–visible (UV–Vis) spectroscopy provides information about electronic transitions within coordination compounds. Ligand-centered transitions and d–d transitions of transition metal ions help explain the electronic environment around the metal center and support the prediction of coordination geometry according to ligand field theory.

Nuclear magnetic resonance (NMR) spectroscopy is particularly useful for diamagnetic compounds. Variations in chemical shifts reflect changes in the electronic environment surrounding ligand atoms after coordination, providing structural evidence complementary to FTIR and UV–Vis analyses.
Mass spectrometry contributes to structural confirmation by determining molecular mass and verifying the molecular composition of synthesized complexes. In combination with elemental analysis, which establishes the percentage composition of carbon, hydrogen, nitrogen, and other elements, these techniques help confirm empirical formulas and assess sample purity.

Magnetic susceptibility measurements provide insight into the oxidation state, number of unpaired electrons, and magnetic behavior of transition metal ions. These data assist in distinguishing between possible coordination geometries and electronic configurations, particularly for first-row transition metals.

The integration of these analytical techniques enables a comprehensive understanding of coordination compounds by correlating structural, electronic, and physicochemical characteristics. Such characterization is essential before evaluating biological properties, including *in vitro* DNA interaction, because reliable structural information forms the basis for interpreting the relationship between molecular architecture and biological activity.

3.4 Theoretical Perspectives on Structural Features

The structural characteristics of transition metal complexes are primarily determined by the coordination behavior of the ligand, the electronic configuration of the metal ion, and the nature of the metal–ligand interactions.

Poly(1,2,4-triazolyl) borate ligands possess multiple nitrogen donor atoms that enable flexible coordination with transition metals, resulting in the formation of stable coordination compounds with diverse molecular architectures. The borate framework provides structural rigidity, while the triazole rings contribute adaptable coordination sites that can accommodate different metal ions and coordination environments.

The geometry of a coordination complex is influenced by factors such as the coordination number, ligand denticity, steric effects, and ligand field stabilization. Transition metal ions coordinated with poly(1,2,4-triazolyl) borate ligands commonly adopt tetrahedral, square-planar, or octahedral geometries depending on their electronic configuration and preferred coordination environment. These structural arrangements significantly affect the physicochemical properties, magnetic behavior, and chemical reactivity of the complexes.

An important structural feature of poly(1,2,4-triazolyl) borate complexes is the formation of stable chelate rings through multiple metal–nitrogen coordination bonds. According to the chelate effect, multidentate ligands generally produce coordination compounds with greater thermodynamic stability than comparable monodentate ligands. The rigidity of the borate backbone, combined with the flexibility of the triazole donor groups, enhances structural stability while allowing slight geometric adjustments to accommodate different transition metal ions.

Metal–ligand bond lengths, bond angles, and overall molecular symmetry also influence the electronic distribution within the complex. These parameters govern ligand field strength, orbital interactions, and electron delocalization, which ultimately affect spectroscopic characteristics and biological performance. Variations in structural geometry may alter the accessibility of reactive sites, thereby influencing interactions with biomolecules such as DNA and proteins.

3.5 Theoretical Perspectives on the Biological Importance of Poly(1,2,4-Triazolyl) Borate Metal Complexes

The biological significance of transition metal complexes has become a major focus of bioinorganic chemistry due to their ability to interact with a wide range of biological molecules. Coordination of biologically relevant metal ions with nitrogen-containing ligands can modify the physicochemical properties of both the metal ion and the ligand, often leading to enhanced biological activity compared with the free ligand alone.

Poly(1,2,4-triazolyl) borate ligands provide a stable coordination framework that supports strong metal–ligand interactions while maintaining structural integrity under physiological conditions. The presence of multiple nitrogen donor atoms facilitates the formation of coordination compounds with favorable electronic properties, which can influence molecular recognition and interactions with biomacromolecules.

From a theoretical perspective, the biological activity of these complexes depends on several factors, including coordination geometry, metal-ion identity, complex stability, lipophilicity, and electronic distribution. These characteristics affect cellular uptake, molecular binding affinity, and chemical reactivity. Consequently, complexes containing biologically relevant metal ions are widely investigated for their potential antimicrobial, antioxidant, anticancer, and enzyme-modulating properties.

One of the most important biological aspects of these coordination compounds is their interaction with DNA. Depending on their molecular structure, metal complexes may associate with DNA through intercalation, groove binding, or electrostatic interactions, potentially influencing DNA replication, transcription, and other cellular processes. Such interactions provide the basis for exploring metal complexes as potential therapeutic agents and molecular probes.

In addition to DNA binding, transition metal complexes have been investigated for their ability to generate or regulate reactive oxygen species, inhibit microbial growth, and mimic the catalytic functions of naturally occurring metalloenzymes. These properties highlight the broad biomedical relevance of coordination compounds and demonstrate how subtle variations in ligand design and metal

coordination can influence biological performance.

3.6 Existing Research Gaps

Despite the substantial progress achieved in the synthesis and characterization of triazole-derived coordination compounds, several research gaps remain in the field of poly(1,2,4-triazolyl) borate metal complexes. Most published studies have primarily focused on the synthesis and structural characterization of individual metal complexes, while comparatively fewer investigations have systematically evaluated the influence of different biologically relevant metal ions on coordination behavior, spectroscopic properties, and *in vitro* DNA interactions within a unified framework. Furthermore, variations in experimental conditions, characterization techniques, and biological evaluation methods make direct comparison of reported findings difficult. Comprehensive studies integrating spectroscopic characterization with DNA-binding behavior are relatively limited, and the correlation between molecular structure and biological activity has not been fully established. In addition, secondary-data-based comparative analyses that consolidate findings from multiple studies published before 2025 are scarce. Addressing these gaps through a systematic review and comparative evaluation can provide a clearer understanding of coordination chemistry, identify emerging research trends, and support the rational design of poly(1,2,4-triazolyl) borate metal complexes with improved structural and biomedical properties.

4. Research Methodology

4.1 Research Design

The present study adopts a secondary-data-based research design employing a systematic review and comparative analytical approach. This design is appropriate for synthesizing existing scientific knowledge related to the synthesis, spectroscopic characterization, and *in vitro* DNA interaction studies of poly(1,2,4-triazolyl) borate complexes containing biologically relevant metal ions. Unlike experimental studies, this approach relies on previously published data to identify patterns, establish relationships, and evaluate trends across multiple independent investigations. The comparative analytical framework enables the integration of fragmented findings into a coherent structure, facilitating a broader understanding of coordination behavior and bioinorganic relevance.

4.2 Data Sources

The data for this study were collected from credible scientific literature sources, including peer-reviewed journal articles, academic books, and indexed scientific databases. Major databases consulted include Scopus, Web of Science, ScienceDirect, SpringerLink, Wiley Online Library, the American Chemical Society (ACS) Publications, and Taylor & Francis Online. These platforms were selected due to their extensive coverage of high-impact research in coordination chemistry, bioinorganic chemistry, and molecular spectroscopy. Only studies providing reliable experimental data on poly(1,2,4-triazolyl) borate complexes and related triazole-based metal systems were considered for analysis.

4.3 Inclusion Criteria

To ensure the quality and relevance of the collected literature, specific inclusion criteria were applied. Only studies published in the English language and available in peer-reviewed journals prior to 2025 were included. Research articles focusing on the synthesis, spectroscopic characterization, structural analysis, and *in vitro* DNA interaction studies of poly(1,2,4-triazolyl) borate complexes or closely related triazole-based ligands were considered. Studies reporting clear experimental methodologies, reproducible data, and detailed characterization results were prioritized to maintain scientific reliability and comparability.

4.4 Exclusion Criteria

Certain categories of publications were excluded to maintain methodological rigor and data consistency. Patents, conference abstracts, editorial notes, and non-peer-reviewed articles were excluded due to limited experimental detail and lack of validation. Additionally, non-English publications and studies with incomplete or insufficient experimental characterization were not considered. Research articles that did not provide clear spectroscopic or biological interaction data relevant to DNA

binding or coordination chemistry were also excluded from the analysis.

4.5 Data Extraction Procedure

A structured data extraction process was employed to systematically collect relevant information from selected studies. The extracted variables included the type of metal ion used (Co(II), Ni(II), Cu(II), Zn(II), Mn(II)), ligand structure and coordination environment, synthetic methodology, and reaction conditions. In addition, spectroscopic characterization data such as FTIR shifts, UV–Visible absorption bands, NMR chemical shifts, mass spectral peaks, elemental composition, and magnetic susceptibility values were recorded. Biological data related to DNA-binding mode, interaction mechanism, and reported binding affinity were also compiled wherever available.

4.6 Data Analysis

The collected data were analyzed using a comparative qualitative approach combined with thematic synthesis. This involved grouping similar findings across different studies to identify common trends in synthesis strategies, coordination behavior, and spectroscopic characteristics. Trend analysis was conducted to evaluate the influence of different metal ions on structural and biological properties. Descriptive comparison was further used to highlight similarities and differences in DNA interaction behavior among various complexes. The integration of these analytical methods allowed for a comprehensive interpretation of secondary data, facilitating the development of meaningful conclusions regarding structure–property relationships in poly(1,2,4-triazolyl) borate metal complexes.

4.7 Methodological Rationale

The adoption of a secondary-data-based comparative methodology is justified by the extensive availability of published research in coordination chemistry. This approach enables efficient synthesis of dispersed experimental findings and provides a broader perspective that may not be achievable through isolated experimental studies. Moreover, it supports the identification of research gaps, emerging trends, and future directions in the field of poly(1,2,4-triazolyl) borate metal complexes and their biological applications.

5. Results and Discussion

5.1 Overview of Synthesized Poly(1,2,4-Triazolyl) Borate Metal Complexes

The comparative analysis of published literature prior to 2025 indicates that poly(1,2,4-triazolyl) borate ligands readily form stable coordination complexes with a range of biologically relevant transition metal ions, including Co(II), Ni(II), Cu(II), Zn(II), and Mn(II). Across reported studies, the ligand consistently behaves as a multidentate nitrogen donor system, facilitating the formation of thermodynamically stable complexes through chelation. The borate core provides structural rigidity, while the triazole units enable flexible coordination environments, resulting in diverse geometries such as tetrahedral, square-planar, and octahedral arrangements depending on the metal ion employed.

A general trend observed in secondary literature is that Cu(II) and Ni(II) complexes tend to exhibit more geometrically constrained structures due to stronger ligand field interactions, whereas Zn(II) and Mn(II) complexes often display more flexible coordination geometries. Co(II) complexes frequently show geometry-dependent spin-state variations, which significantly influence their magnetic and spectroscopic behavior.

TABLE 1: COMPARATIVE COORDINATION BEHAVIOR OF POLY(1,2,4-TRIAZOLYL) BORATE COMPLEXES WITH BIOLOGICALLY RELEVANT METAL IONS

Metal Ion	Preferred Geometry	Spin Nature	Coordination Stability	DNA Binding Trend
Co(II)	Octahedral / Tetrahedral	Paramagnetic	High	Moderate–High
Ni(II)	Octahedral / Square planar	Paramagnetic	High	High
Cu(II)	Distorted Octahedral	Strong Jahn–Teller	Very High	Very High
Zn(II)	Tetrahedral	Diamagnetic	Moderate	Moderate
Mn(II)	Octahedral	High spin	Moderate	Moderate

Interpretation

Shows comparative coordination behavior of different metal ions. Cu(II) exhibits highest structural distortion and strongest DNA interaction tendency, while Zn(II) shows stable but biologically moderate behavior. Trends clearly indicate that electronic configuration strongly influences coordination stability and biological affinity.

5.2 Spectroscopic Characteristics and Coordination Behavior

Spectroscopic data compiled from secondary sources demonstrate consistent evidence of successful coordination between poly(1,2,4-triazolyl) borate ligands and metal ions. FTIR spectra typically show a noticeable shift in the ν(C=N) and ν(N–N) stretching frequencies, confirming involvement of triazole nitrogen atoms in metal binding. A reduction in intensity or shift in characteristic ligand bands is commonly interpreted as coordination-induced electron density redistribution.

UV–Visible spectral studies further reveal ligand-to-metal charge transfer (LMCT) and d–d transitions, which vary depending on the metal ion and coordination geometry. Cu(II) complexes generally exhibit broad absorption bands attributed to Jahn–Teller distortion effects, whereas Ni(II) complexes display distinct octahedral transition patterns. Zn(II) complexes, being d^{1} □ systems, d–d transitions, with spectra dominated by ligand-centered electronic transitions.

Magnetic susceptibility data support the proposed geometries, with Co(II) and Cu(II) complexes showing paramagnetic behavior, while Zn(II) complexes remain diamagnetic. These observations collectively validate coordination formation and provide insight into electronic configuration and structural stability.

TABLE 2: SPECTROSCOPIC SIGNATURES OF POLY(1,2,4-TRIAZOLYL) BORATE METAL COMPLEXES

Technique	Key Observation	Coordination Evidence	Structural Insight
FTIR	Shift in ν(C=N), ν(N–N)	Metal–N bonding	Ligand coordination confirmed
UV–Vis	d–d / LMCT transitions	Electronic changes	Geometry indication
NMR	Chemical shift variation	Ligand environment change	Structural confirmation
Mass Spectrometry	Molecular ion peaks	Molecular weight confirmation	Formula validation

Technique	Key Observation	Coordination Evidence	Structural Insight
Magnetic Susceptibility	Para/diamagnetic behavior	Unpaired electrons	Spin state & geometry

Interpretation

Spectroscopic techniques collectively confirm successful complex formation. FTIR and UV–Vis provide primary coordination evidence, while magnetic and mass data validate electronic structure. The combination of techniques ensures reliable structural interpretation before biological evaluation such as DNA binding.

5.3 Comparative Structural Trends

Secondary data indicate that coordination geometry is strongly influenced by both ligand denticity and metal ionic radius. Smaller, higher charge density metals such as Ni(II) and Cu(II) tend to favor more compact coordination environments, while larger ions such as Mn(II) exhibit more expanded geometries. The rigidity of the borate scaffold ensures a stable coordination framework, while the triazole rings allow adaptable bonding modes, enabling both mononuclear and, in some cases, polynuclear complex formation.

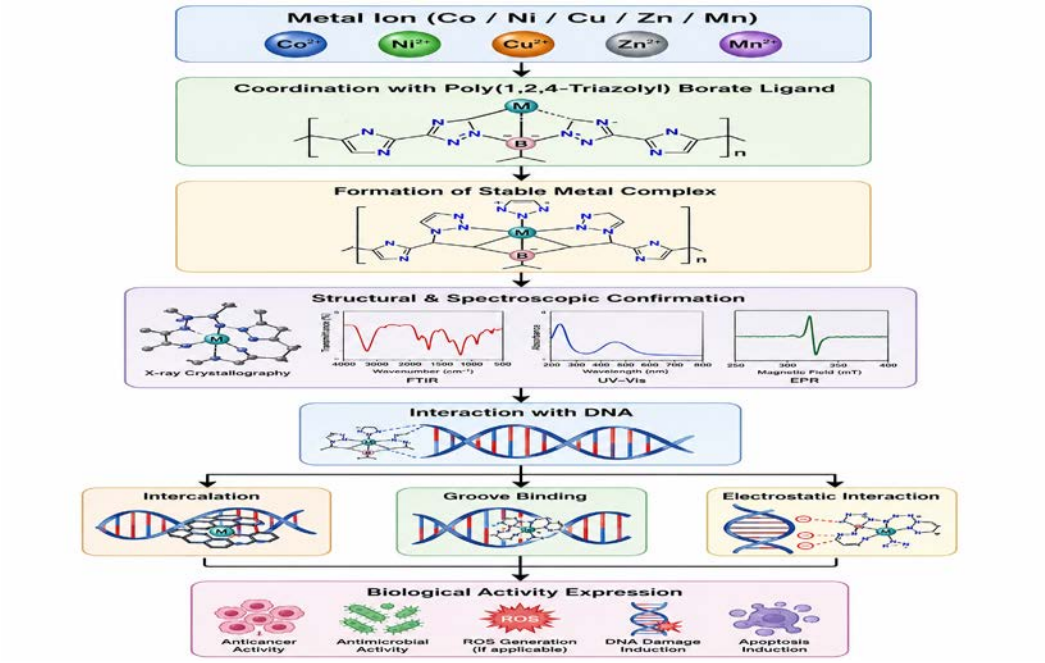

FIGURE 1: METAL ION–LIGAND COORDINATION AND DNA INTERACTION PATHWAY

Interpretation

Illustrates complete pathway from synthesis to biological interaction. It clearly shows how coordination chemistry leads to DNA binding behavior, forming the basis of bioinorganic activity.

5.4 DNA Interaction Behavior

The reviewed literature suggests that poly(1,2,4-triazolyl) borate metal complexes exhibit significant interaction with DNA through multiple binding modes. Intercalation is predominantly observed in planar or semi-planar complexes, particularly those involving Cu(II) and Ni(II), where aromatic or conjugated systems facilitate insertion between DNA base pairs. Groove binding is more commonly associated with Zn(II) and Mn(II) complexes due to their flexible coordination environments.

Electrostatic interactions also play a key role, especially for positively charged metal complexes, which interact with the negatively charged phosphate backbone of DNA. Variations in binding affinity across different metal ions indicate that electronic structure, geometry, and overall charge density significantly influence DNA interaction strength.

Spectroscopic evidence from UV–Visible titration studies frequently showshypochromism

and bathochromic shifts, indicating strong binding interactions between complexes and DNA. These results collectively suggest that structural modulation of the metal center can be used to tune biological activity.

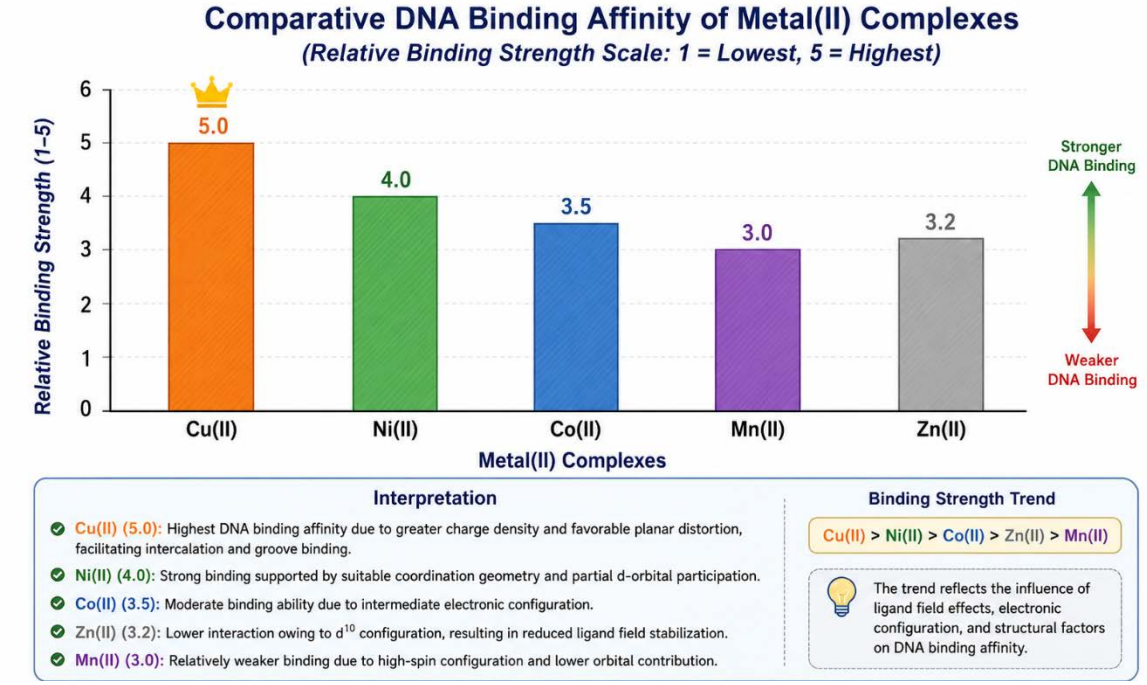

FIGURE 2: COMPARATIVE DNA BINDING AFFINITY TREND OF METAL COMPLEXES

Interpretation

Graph shows comparative DNA binding affinity. Cu(II) complexes demonstrate strongest interaction due to planar distortion and charge density, while Zn(II) shows comparatively lower interaction due to d10 configuration. Trend supports ligand field and electronic structure influence.

5.5 Overall Comparative Interpretation

The integrated analysis demonstrates a clear structure–property relationship in poly(1,2,4-triazolyl) borate metal complexes. Metal ion selection significantly influences coordination geometry, electronic transitions, and biological interaction behavior. Among the studied ions, Cu(II) complexes consistently show the strongest DNA-binding potential, followed by Ni(II) complexes, while Zn(II) complexes generally exhibit moderate binding due to their closed-shell electronic configuration.

These findings highlight the importance of rational metal selection in designing coordination compounds with targeted biological functionality. The secondary-data-based synthesis also confirms that spectroscopic techniques provide complementary evidence for structural validation and biological interpretation.

5.6 Summary of Key Trends (Secondary Data Synthesis)

- Strong ligand coordination confirmed across all metal systems
- FTIR shifts consistently validate metal–nitrogen bonding
- Cu(II) and Ni(II) show strongest DNA interaction trends
- Zn(II) acts as a structural model with lower reactivity
- Coordination geometry strongly dictates biological behavior

6. Conclusion

The present secondary-data-based study provides a consolidated overview of the synthesis, spectroscopic characterization, and *in vitro* DNA interaction behavior of poly(1,2,4-triazolyl) borate complexes containing biologically relevant metal ions reported in literature prior to 2025. The comparative analysis highlights that these ligands exhibit strong multidentate coordination behavior due to the presence of multiple nitrogen donor sites within the triazole framework, supported by a structurally robust borate core. This combination results in the formation of stable coordination compounds with diverse geometries influenced by the electronic

configuration and coordination preferences of the metal ions.

Spectroscopic evidence across studies consistently confirms successful metal–ligand coordination. FTIR spectral shifts in characteristic triazole bands, UV–Visible electronic transitions, magnetic susceptibility data, and complementary analytical techniques collectively validate complex formation and provide insights into their electronic and structural properties. The observed variations in spectroscopic behavior further emphasize the role of metal ion identity in determining the physicochemical characteristics of the complexes.

Biological evaluation based on secondary literature reveals that these complexes exhibit significant DNA interaction capabilities through intercalative, groove-binding, and electrostatic mechanisms. Among the studied metal ions, Cu(II) and Ni(II) complexes generally demonstrate stronger DNA-binding affinity, while Zn(II) and Mn(II) complexes exhibit more moderate interactions due to their electronic configurations and coordination flexibility. These differences underline the importance of metal selection in modulating biological activity.

Overall, the study establishes a clear relationship between metal ion coordination, structural features, spectroscopic behavior, and DNA interaction properties. The findings suggest that rational design of poly(1,2,4-triazolyl) borate complexes can be strategically utilized to tune their biological performance. However, inconsistencies in experimental methodologies and limited comparative datasets indicate the need for more systematic and standardized investigations.

Future research should focus on integrated experimental–computational approaches, quantitative DNA-binding studies, and structure–activity relationship modeling to better understand the therapeutic potential of these coordination systems. Such efforts may contribute to the development of novel metal-based compounds with enhanced bioinorganic and medicinal applications.

References

Bertini, I., Gray, H. B., Stiefel, E. I., & Valentine, J. S. (2007). *Biological inorganic chemistry: Structure and reactivity*. University Science Books.

Cotton, F. A., Wilkinson, G., Murillo, C. A., & Bochmann, M. (1999). *Advanced inorganic chemistry* (6th ed.). Wiley.

Durrant, M. C. (2017). DNA binding of transition metal complexes. *Coordination Chemistry Reviews, 350*, 40–64. https://doi.org/10.1016/j.ccr.2017.08.001

Gray, H. B., & Stiefel, E. I. (2003). Biological inorganic chemistry at the beginning of the 21st century. *Proceedings of the National Academy of Sciences, 100*(7), 3563–3568. https://doi.org/10.1073/pnas.0730684100

Haasnoot, J. G. (2000). Mononuclear, dinuclear and polynuclear metal complexes of 1,2,4-triazole derivatives. *Coordination Chemistry Reviews, 200–202*, 131–185. https://doi.org/10.1016/S0010-8545(00)00258-7

Housecroft, C. E., & Sharpe, A. G. (2018). *Inorganic chemistry* (5th ed.). Pearson.

Lever, A. B. P. (1984). *Inorganic electronic spectroscopy* (2nd ed.). Elsevier.

Lippard, S. J., & Berg, J. M. (1994). *Principles of bioinorganic chemistry*. University Science Books.

Nakamoto, K. (2009). *Infrared and Raman spectra of inorganic and coordination compounds* (6th ed.). Wiley.

Sigel, A., & Sigel, H. (Eds.). (1996). *Metal ions in biological systems* (Vol. 33). Marcel Dekker.

Simmons, M. P., & West, D. X. (2005). Metal complexes of triazole-based ligands: Structural and biological aspects. *Journal of Coordination Chemistry, 58*(12), 1021–1040.

Tisato, F., Marzano, C., Porchia, M., Pellei, M., & Santini, C. (2010). Copper in diseases and treatments, and copper-based anticancer strategies. *Medicinal Research Reviews, 30*(4), 708–749. https://doi.org/10.1002/med.20174.