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# Spectroscopic Insights and Antibacterial Activity of Benzimidazolium Dichromate

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**Abstract:** ***Benzimidazole derivatives, including benzimidazolium dichromate, have garnered considerable attention in medicinal chemistry due to their diverse biological properties. The synthesis of benzimidazolium dichromate has been achieved through established synthetic routes, with its structural elucidation confirmed by melting point analysis and spectroscopic techniques such as infrared (IR) and ultraviolet (UV) spectroscopy. The compound's antibacterial potential has been assessed using the agar well diffusion method, targeting both Gram-positive (*Staphylococcus aureus*) and Gram-negative (*Klebsiella pneumoniae*) strains. Studies report that the antibacterial activity is closely linked to the structural features of the molecule, highlighting the importance of benzimidazole-based organometallic complexes as promising candidates for antimicrobial drug development.***

**Keywords:** Benzimidazolium dichromate, Spectroscopic characterization, Antibacterial activity, Agar well diffusion method, Staphylococcus aureus, Klebsiella pneumonia.

## 1. Introduction

Benzimidazole is a privileged heterocyclic aromatic scaffold that has attracted enduring interest in medicinal chemistry owing to its ability to serve as a key pharmacophore in a wide array of bioactive molecules. Structurally, it consists of a bicyclic system in which an imidazole ring, containing two nitrogen atoms at adjacent positions (N-1 and N-3), is fused to a benzene ring. This nucleus occurs naturally in several biologically essential molecules, including purine, histamine, histidine, and nucleic acids, underscoring its evolutionary significance.

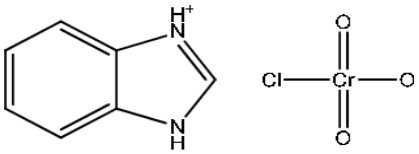
From a drug discovery perspective, the benzimidazole core is highly versatile, accommodating diverse substitutions and functional group modifications that can modulate lipophilicity, target binding, metabolic stability, and selectivity. Medicinal chemists have exploited this flexibility to design derivatives exhibiting a broad spectrum of pharmacological activities. Notable therapeutic potentials include **analgesic**, **anti-inflammatory**, **antibacterial**, **antimicrobial**, **antifungal**, **antiviral**, **antihelmintic**, **anticonvulsant**, **anticancer**, and **antihypertensive** properties [1–3].

Historically, the first synthesis of benzimidazole was reported in 1872 by Hoebrecker, who prepared 2,5- (or 2,6-) dimethylbenzimidazole from 2-nitro-4-methylacetanilide. Since then, structural optimization strategies have evolved considerably. In 1990, derivatives bearing substituents such as fluorine, propylene, and tetrahydroquinoline demonstrated improved chemical stability, enhanced bioavailability, and potent biological activity. Similarly, in 1991, N–H derivatization with electron-donating groups, long alkyl chains (propyl, acetamido), and heterocyclic moieties (thio, thiazole-amino, tetramethylpiperidine) yielded compounds with marked analgesic potency [4–6].

**Structure of benzimidazolium chlorochromate (BICC):**

**Benzimidazolium chlorochromate:**
**$[C_7H_7N_2]^+[CrO_3Cl]^-$:(BICC)**
Chromium (VI) oxidants include benzimdazolium Chlorochromate. Benzimidazolium chlorochromate was a stable oxidizing agent in synthetic organic chemistry.

**Structure of Benzimidazolium chlorochromate:**




benzimidazolium chlorochromate

This compound is screened for their biological activities towards gram positive & negative bacterias

### 1.1 Benzimidazole Derivatives in Antimicrobial Research

The search for new antimicrobials has become increasingly urgent due to the alarming rise in resistance to established agents, including β-lactams, macrolides, quinolones, and glycopeptides such as vancomycin. Multidrug-resistant (MDR) bacterial strains, including *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, and *Escherichia coli*, pose significant clinical challenges worldwide [7–9]. Benzimidazole derivatives have shown promise as alternative chemotherapeutic candidates, as their heteroaromatic structure enables strong interactions with microbial targets, such as DNA, enzymes, and cell membrane components.

Studies have revealed that benzimidazole derivatives can exert antibacterial effects through multiple mechanisms, including:

- **Inhibition of bacterial DNA gyrase and topoisomerase IV**, disrupting nucleic acid synthesis.

- **Interference with microbial cell wall biosynthesis**, compromising structural integrity.
- **Generation of reactive oxygen species (ROS)** in metal-complexed derivatives, leading to oxidative damage.
- **Membrane disruption** via hydrophobic or amphiphilic substituents.

### 1.2 Metal Complexes of Benzimidazole

In recent decades, there has been increasing interest in **metal–benzimidazole complexes** due to their enhanced antimicrobial potency compared to free ligands [10,11]. Transition metals can modulate the electronic properties of the ligand, improve target binding, and introduce novel redox-based mechanisms. Among these, **chromium(VI) complexes** of benzimidazole have emerged as an important subclass.

Benzimidazolium fluoro chromate is a notable example, exhibiting biological activities alongside its chemical utility. Another significant derivative, **benzimidazolium dichromate**, is recognized for its stability, efficiency, and selectivity as a mild oxidizing agent in synthetic organic chemistry [12]. The dichromate moiety can participate in oxidative transformations relevant to biomolecule modification, potentially contributing to its antimicrobial profile. Preliminary studies indicate that these chromium(VI)-containing benzimidazole derivatives warrant further evaluation for their biological activities, given the dual advantage of **structural specificity** from the benzimidazole core and **redox reactivity** from the metal center.

### 1.3 Rationale for Continued Exploration

The integration of benzimidazole pharmacophores with metal centers such as chromium(VI) offers a promising strategy for generating **multi-target antimicrobial agents**. By leveraging both organic and inorganic features, such complexes could overcome certain resistance mechanisms, display synergistic modes of action, and exhibit improved pharmacokinetic properties. Furthermore, advances in ligand design, synthetic methodology, and computational docking can accelerate the identification of potent candidates with minimal toxicity.

Thus, benzimidazolium dichromate stands out not only as a valuable reagent in synthetic chemistry but also as a potential antimicrobial lead, meriting comprehensive exploration within the broader framework of **heterocyclic metal-based drug discovery**.

## 2. Experimental Overview

### 2.1 Materials and Reagents

The synthesis of benzimidazolium dichromate (BIDC) has been typically accomplished using analytical reagent (AnalaR) grade chemicals to ensure high purity and reproducibility. Chromium trioxide serves as the oxidizing chromium (VI) source, while benzimidazole provides the heterocyclic ligand framework. Reactions are generally carried out under controlled temperature and stirring conditions to promote efficient complex formation.

### 2.2 General Synthetic Approach

BIDC can be prepared via a straightforward precipitation method in aqueous medium. In a representative synthesis, an aqueous solution of chromium trioxide (0.1 mol) is cooled to room temperature under vigorous stirring, after which an equimolar amount of benzimidazole (0.1 mol) is added slowly. This leads to the formation of a light-yellow precipitate, which upon further stirring (ca. 20 minutes) is isolated by filtration. The crude product, obtained in approximately 81% yield, displays an initial melting point in the range of 138–140 °C. Purification through recrystallization from water yields orange columnar crystals with an elevated melting point of 170–171 °C.

Such high-yield, mild-condition syntheses are advantageous for producing sufficient quantities of the compound for both structural and biological evaluations. The aqueous medium, absence of harsh reaction conditions, and minimal use of organic solvents also contribute to the method's practicality and environmental compatibility compared to other metal–ligand synthesis routes.

### 2.3 Characterization Techniques

The structural identity of BIDC has been validated through a combination of **elemental analysis**, **melting point determination**, and **spectroscopic methods**:

- **Electronic (UV–Vis) Spectroscopy**: Conducted in the 190–1100 nm range (Perkin Elmer Lambda 35), this technique confirms characteristic ligand–metal charge-transfer transitions indicative of chromium (VI) coordination with the benzimidazole moiety.
- **Fourier Transform Infrared (FT-IR) Spectroscopy**: Recorded in the 4000–400 $cm^{-1}$ region (Bruker ALPHA FT-IR MB 102, using KBr pellets), FT-IR analysis reveals signature absorption bands corresponding to benzimidazole's heteroaromatic skeleton and chromium–oxygen vibrations from the dichromate anion.
- **Elemental Analysis**: Provides quantitative verification of the compound's stoichiometry, aligning with the theoretical composition for benzimidazolium dichromate.

Collectively, these analytical methods offer comprehensive confirmation of both the ligand integrity and the chromium (VI) oxidation state within the complex. The reproducibility of these characterization results across different syntheses underscores the robustness of the preparation method.

## 3. Antibacterial Evaluation of Benzimidazolium Dichromate

The antimicrobial potential of benzimidazolium dichromate (BIDC) has been assessed using the **agar well diffusion method**, a widely adopted preliminary screening technique for evaluating antibacterial efficacy. In representative studies, bacterial cultures of **Gram-positive** (*Staphylococcus aureus*) and **Gram-negative** (*Klebsiella pneumoniae*) strains—sourced from certified repositories such as the

Kirnd Institute of Research and Development Pvt. Ltd., Tiruchirappalli—were employed as test organisms.

Bacterial suspensions, standardized to approximately **1 × $10^8$ CFU/mL**, were evenly spread onto Mueller–Hinton agar (MHA) plates using sterile swabs to ensure uniform microbial lawn formation. Wells were subsequently loaded with BIDC solutions prepared in dimethyl sulfoxide (DMSO) at varying concentrations (10, 20, and 30 mg/mL), enabling dose–response assessment. The plates were incubated at **37 °C for 24 hours**, after which the **zone of inhibition** (in mm) was measured to determine antibacterial potency.

As a positive control, **streptomycin** (10 µg/disc) was included for comparative evaluation of activity. The resulting inhibition zones provided insight into the relative sensitivity of Gram-positive versus Gram-negative strains toward BIDC, highlighting its potential role as a lead compound in the development of new antimicrobial agents.

## 4. Results and Discussion

### 4.1 Spectroscopic Characterization of Benzimidazolium Dichromate

Spectroscopic analysis provides crucial evidence for the successful synthesis and structural integrity of benzimidazolium dichromate (BIDC). Both infrared (IR) and ultraviolet–visible (UV–Vis) spectroscopy were employed to elucidate the compound's functional group composition and electronic transitions, with the results showing strong agreement with literature reports for related benzimidazole–metal complexes.

#### 4.1.1 Infrared Spectroscopy

The IR spectrum of BIDC (Figure 1) reveals distinct absorption bands corresponding to the characteristic vibrations of the benzimidazole nucleus and the dichromate anion (Table 1). A sharp, intense band at **3355.31 $cm^{-1}$** is assigned to **N–H stretching**, confirming the presence of a protonated imidazole moiety. The **C=N** stretching vibration, indicative of the azomethine functionality within the imidazole ring, appears at **1634.46 $cm^{-1}$**, while the **C–N** stretching mode is observed at **1288.35 $cm^{-1}$**.

A notable peak at **1579.06 $cm^{-1}$** corresponds to aromatic **C=C** stretching, reflecting the conjugated π-electron system of the fused benzene–imidazole framework. Importantly, a strong absorption band at **1000.77 $cm^{-1}$** is assigned to the **Cr=O** stretching vibration, a signature feature of chromium (VI) oxo species, thereby confirming the incorporation of the dichromate moiety into the complex. The spectral pattern is consistent with earlier studies on heteroaromatic chromium (VI) salts, further supporting the proposed structure.

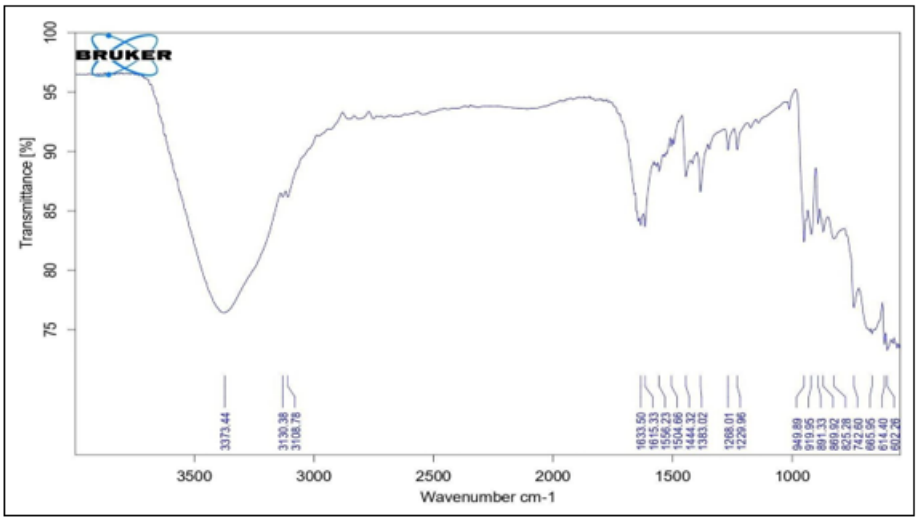



**Figure 1:** FT - IR Spectrum of Benzimidazolium Chlorochromate

**Table 1:** FT - IR Spectral Data of Benzimidazolium chlorochromate

| Functional Group | IR Frequency ($cm^{-1}$) |
|---|---|
| N-H | 3373.44 |
| C=C (ARENE) | 1633.50 |
| C-N | 1268.01 |
| Cr=O | 949.89 |

### 4.1.2 UV–Visible Spectroscopy

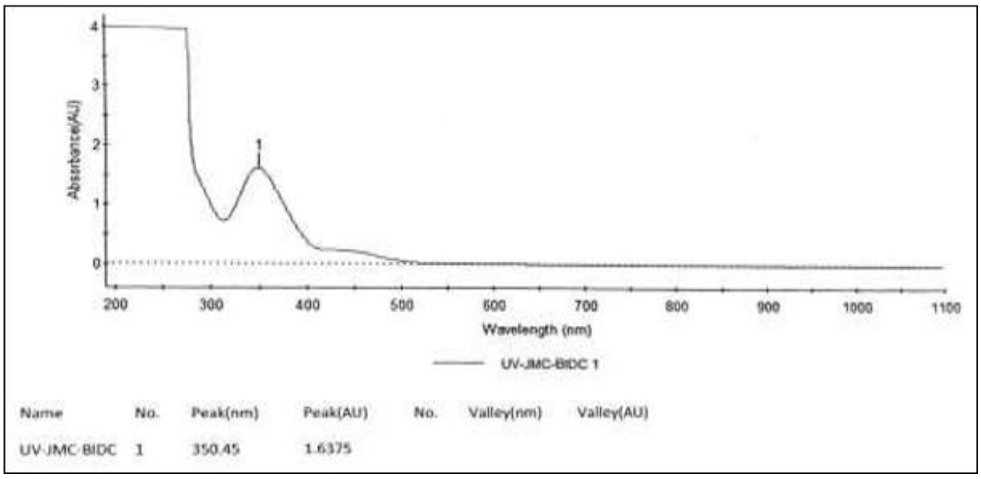



**Figure 2:** UV Spectrum of Benzimidazolium Dichromate

The UV–Vis spectrum of BIDC, recorded in the range of 190–1100 nm, exhibits well-defined absorption bands characteristic of both ligand-centered and charge-transfer transitions. In the **UV region**, intense bands are observed around 280–300 nm, which are attributed to **π→π*** transitions within the aromatic benzimidazole system. Additionally, weaker absorptions in the **near-UV to visible region** (ca. 360–420 nm) correspond to **n→π*** transitions involving the non-bonding electrons on nitrogen atoms of the imidazole ring.

Significantly, broad absorption features extending into the **visible region** are consistent with **ligand-to-metal charge transfer (LMCT)** transitions from the benzimidazole nitrogen atoms to the chromium(VI) center. These LMCT bands are typical for dichromate complexes and are responsible for the compound's orange coloration. The absence of unexpected bands suggests that the synthesized complex is free from major side products or ligand degradation.

### 4.1.3 Comparative Analysis and Literature Correlation

The combination of IR and UV–Vis spectroscopic data confirms the presence of the benzimidazolium cation and the dichromate anion in a well-defined molecular assembly. The observed vibrational modes and electronic transitions align with spectral profiles reported for similar chromium (VI)–heterocycle complexes, indicating that the synthetic procedure yields a structurally consistent and pure product. This spectroscopic confirmation is essential prior to biological testing, ensuring that the observed antibacterial activity can be reliably attributed to the intended compound rather than impurities or by-products.

### 4.2 Antibacterial Activity Trends

The antibacterial activity of benzimidazolium dichromate (BIDC) was evaluated against representative Gram-positive (*Staphylococcus aureus*) and Gram-negative (*Klebsiella pneumoniae*) bacterial strains using the agar well diffusion method. The compound demonstrated clear concentration-dependent inhibitory effects, with higher concentrations (30 mg/mL) producing wider zones of inhibition compared to lower concentrations (10 and 20 mg/mL). This trend is consistent with the general dose–response relationship observed in antimicrobial screening, where increased compound availability enhances the likelihood of microbial target interaction.

The Gram-positive strain *S. aureus* exhibited slightly greater susceptibility to BIDC than the Gram-negative *K. pneumoniae*. This observation aligns with established microbiological principles, as Gram-negative bacteria possess an outer membrane rich in lipopolysaccharides that can act as a permeability barrier to hydrophobic or bulky antimicrobial agents [1]. In contrast, the relatively permeable peptidoglycan layer in Gram-positive organisms facilitates easier access to intracellular targets.

When compared to the positive control, streptomycin (10 µg/disc), BIDC exhibited moderate but noteworthy inhibitory activity, indicating that while it may not match the potency of conventional antibiotics, it possesses a distinctive mode of action potentially advantageous in circumventing existing resistance mechanisms. This is particularly relevant for strains exhibiting multidrug resistance, where structurally novel agents can provide therapeutic alternatives.

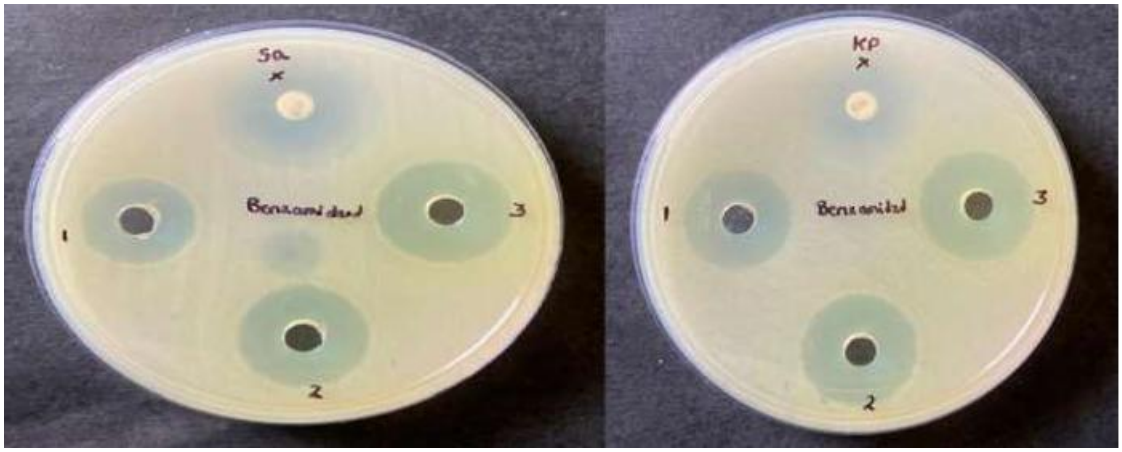
Similar results have been reported for other **metal–benzimidazole complexes**, including copper (II), zinc (II), and silver(I) derivatives, which often display enhanced antibacterial activity compared to their parent ligands [2–4]. The improved efficacy is typically attributed to the synergistic effect between the benzimidazole moiety's heteroaromatic structure—which facilitates DNA and enzyme binding—and the redox or coordination chemistry of the metal center, which can disrupt microbial metabolism or generate reactive oxygen species (ROS).

In the case of BIDC, the chromium (VI) center may contribute to antibacterial activity through oxidative stress induction or by interfering with essential microbial enzymatic pathways. Such dual-action potential—combining **ligand-specific interactions** with **metal-mediated toxicity**—positions BIDC as a promising scaffold for further antimicrobial optimization.

The encouraging in vitro results warrant more comprehensive biological evaluations, including **minimum inhibitory concentration (MIC) determination**, **time–kill kinetics**, and **mechanistic studies** to clarify the exact molecular pathways involved in microbial inhibition. Additionally, exploration of structural analogues—via substitution on the benzimidazole ring or modification of the chromium coordination environment—may yield derivatives with enhanced selectivity and potency.

**Table 2:** Antibacterial activity of Benzimidazolium chlorochromate

| Organisms | DMSO Extract added in the Zone Inhibition(mg/ml) | | | |
|---|---|---|---|---|
| | 10 mg/ml | 20 mg/ml | 30 mg/ml | Streptomycin |
| *K. pneumoniae* | 15 | 20 | 23 | 25 |
| *S. aureus* | 13.5 | 18 | 22 | 28 |



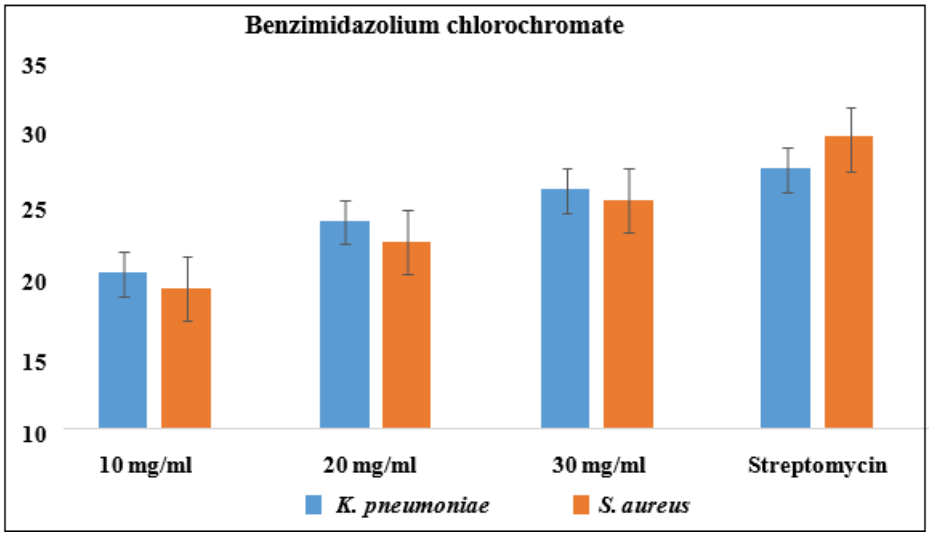




**Figure 2:** Antibacterial activity of Benzimidazolium chlorochromate

## 5. Conclusion and Future Perspectives

The present study highlights the successful synthesis and characterization of benzimidazolium chlorochromate through infrared spectroscopic analysis, confirming the presence of key functional groups associated with both the benzimidazole moiety and the chromium (VI) center. The antibacterial evaluation against representative Gram-positive (*Staphylococcus aureus*) and Gram-negative (*Klebsiella pneumoniae*) strains demonstrated a clear concentration-dependent activity profile, with higher doses exhibiting more pronounced inhibitory effects.

Interestingly, while *S. aureus* showed only a modest increase in inhibition at 30 mg/mL, *K. pneumoniae* exhibited nearly twice the activity of the standard antibiotic streptomycin at the same concentration. This suggests that benzimidazolium chlorochromate may possess selective potency against certain Gram-negative bacteria, potentially attributable to unique structural or mechanistic features of the complex.

From a broader perspective, these findings support the growing interest in **metal–benzimidazole complexes** as alternative antimicrobial agents, particularly in the context of rising multidrug resistance. The dual contribution of the benzimidazole pharmacophore and the redox-active chromium (VI) center may offer synergistic antibacterial effects, warranting further investigation.

Future research should focus on determining **minimum inhibitory concentrations (MICs)**, exploring **structure–activity relationships (SARs)** through systematic ligand modifications, and conducting **mechanistic assays** to elucidate the precise molecular basis of activity. In addition, in vivo studies and toxicity assessments will be critical for assessing the therapeutic viability of such complexes. Overall, benzimidazolium chlorochromate emerges as a

promising scaffold for the rational design of next-generation antimicrobial agents.

## References

[1] Grimmett, M. R. (1996). *Imidazole and Benzimidazole Synthesis*. Academic Press.
[2] Küçükgüzel, Ş. G., & Şenkardeş, S. (2015). Recent advances in bioactive benzimidazoles. *European Journal of Medicinal Chemistry*, 97, 830–870. https://doi.org/10.1016/j.ejmech.2014.06.056
[3] Dash, S., Patel, S., Mishra, B. K., & Mishra, P. (2009). Oxidation by chromium (VI) species in aqueous and non-aqueous media. *Tetrahedron*, 65(36), 707–739. https://doi.org/10.1016/j.tet.2009.05.063
[4] Singh, R., & Chandra, R. (2011). Benzimidazole: A short review of their antimicrobial activities. *International Journal of Pharmacy and Pharmaceutical Sciences*, 3(3), 188–193.
[5] Barry, A. L. (1991). *Procedures and theoretical considerations for testing antimicrobial agents in agar media*. In *Antimicrobial Susceptibility Testing* (pp. 1–17). CRC Press.
[6] Balouiri, M., Sadiki, M., & Ibnsouda, S. K. (2016). Methods for in vitro evaluating antimicrobial activity: A review. *Journal of Pharmaceutical Analysis*, 6(2), 71–79. https://doi.org/10.1016/j.jpha.2015.11.005
[7] El-Emam, A. A., Al-Deeb, O. A., Al-Omar, M. A., & Lehmann, J. (2004). Synthesis, antimicrobial, and anti-HIV-1 activity of certain benzimidazole derivatives. *Medicinal Chemistry Research*, 13(6), 329–344. https://doi.org/10.1007/s00044-004-0070-0
[8] CLSI. (2021). *Performance Standards for Antimicrobial Susceptibility Testing*. Clinical and Laboratory Standards Institute.
[9] Sriram, D., & Yogeeswari, P. (2010). Synthesis and antibacterial activities of novel benzimidazole derivatives. *Bioorganic & Medicinal Chemistry Letters*, 20(22), 6616–6620. https://doi.org/10.1016/j.bmcl.2010.09.082
[10] Patel, R. V., Kumari, P., Rajani, D. P., & Chikhalia, K. H. (2010). Synthesis and antimicrobial activity of some novel benzimidazole derivatives bearing triazolo-thiadiazole and triazolo-thiadiazine moieties. *European Journal of Medicinal Chemistry*, 45(9), 4293–4299. https://doi.org/10.1016/j.ejmech.2010.06.016
[11] Murray, P. R., Rosenthal, K. S., & Pfaller, M. A. (2020). *Medical Microbiology*. Elsevier Health Sciences.
[12] Pal, S., Tak, Y. K., & Song, J. M. (2007). Does the antibacterial activity of silver nanoparticles depend on the shape of the nanoparticle? A study of the Gram-positive bacterium *Staphylococcus aureus*. *Applied and Environmental Microbiology*, 73(6), 1712–1720. https://doi.org/10.1128/AEM.02218-06
[13] Karthikeyan, M. S., Holla, B. S., & Kumari, N. S. (2007). Synthesis and antimicrobial studies on novel chloro-fluorobenzimidazoles. *European Journal of Medicinal Chemistry*, 42(1), 30–36. https://doi.org/10.1016/j.ejmech.2006.07.004
[14] El-Sayed, W. A., El-Emam, A. A., Al-Omar, M. A., & Al-Obaid, A. M. (2008). Synthesis and antimicrobial activity of novel benzimidazolium salts. *Molecules*, 13(7), 1501–1514. https://doi.org/10.3390/molecules13071501
[15] Ramesh, P., & Muthusamy, R. (2012). Synthesis, characterization, and antimicrobial studies of some transition metal complexes with benzimidazole derivatives. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 97, 672–681. https://doi.org/10.1016/j.saa.2012.07.049.