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Research Article

Synthesis, Thermal Behavior and Metal Selectivity of New Benzyloxy-Pyridine Compound

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Abstract: In this study, a novel benzyloxy-pyridine derivative, 2-(benzyloxy)-5-bromo-3-nitropyridine (compound **L**), was synthesized from benzyloxy bromide and 2-hydroxy-3-nitro-5-bromopyridine. The synthesized compound (**L**) was characterized by spectroscopic techniques. ^{1}H-NMR data were used to determine the chemical shift values (ppm) of all protons in the compound and the coupling constants (Hz) for the relevant protons. ^{13}C-NMR was used to determine the chemical shift values (ppm) for all carbons. ^{1}H- and ^{13}C-NMR spectra unambiguously supported the proposed molecular structure. FT-IR spectroscopy confirmed the presence of key functional groups through characteristic absorption bands. High-resolution mass spectrometry (HRMS) confirmed the molecular composition clearly, with the observed mass closely matching the calculated value. Thermal properties of compound **L** were investigated under a nitrogen atmosphere at a heating rate of 10 °C min^{-1} using TGA/DTA techniques, revealing good thermal stability up to approximately 300 °C followed by complete decomposition without residue formation. The metal selectivity of compound **L** was evaluated fluorometrically with different metal salts. For this purpose, compound **L** was interacted with alkali metal (Li^{+}, Na^{+}, K^{+}), alkaline earth metal (Mg^{2+}, Ca^{2+}), post-transition metal (Al^{3+}), and transition metal (Cr^{3+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, and Ag^{+}) salts at a concentration of 1:100 (ligand:metal) in ethanol medium. The results show that compound **L** exhibits selectivity with a distinct fluorescence quenching effect toward specific metal ions (Cr^{3+}, Fe^{3+}, and Cu^{2+}).

Keywords: *Synthesis, Spectroscopy, Thermal analysis, Metal selectivity*

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I. INTRODUCTION

Small molecules stand out as fundamental tools in many areas of modern science; they form the basis of many products that directly affect daily life, such as drugs, biological probes, agricultural chemicals, dyes, and functional materials (Trobe & Burke, 2018). Their ability to modulate protein functions makes them essential both in drug discovery and in the investigation of biological processes (Galloway et al., 2010; Schreiber, 2000). This broad scope makes small molecule synthesis one of the most important bridges between chemistry, biology, and drug discovery (Galloway et al., 2010; Mohanasundaram et al., 2021; Schreiber, 2000, 2011).

Metal ions play an important role in biological processes in the human body (A. Kumar et al., 2022; Zheng et al., 2020). Alkali (Na^{+}, K^{+}), alkaline earth (Ca^{2+}, Mg^{2+}), and transition metals (Fe^{2+}/Fe^{3+}, Zn^{2+}, Cu^{2+}) are essential components in maintaining vital processes, including fluid-electrolyte balance, neurotransmission, energy production, gene expression, and structural biomolecular functions (Zheng et al., 2020). Additionally, metal ions such as Cd^{2+}, Hg^{2+}, Pb^{2+}, Mn^{2+}, Pd^{2+}, Cr^{3+}, and Ni^{2+} have an essential part in many industrial processes and can be found in various natural and artificial environments (A. Kumar et al., 2022; Velusamy et al., 2021). However, exposure to these ions has serious adverse effects on both human health and the environment. When taken beyond the permitted limits, they can cause serious health problems, including metabolic disorders, organ damage, neurodegenerative diseases, and various systemic complications (A. Kumar et al., 2022; Kumar Goshisht et al., 2022; Onursal, 2026). Therefore, the detection of metal ions is of great importance.

Various studies in the literature describe the use of heteroatom-containing cyclic and aromatic compounds in the fluorometric determination of metal ions (A. Kumar et al., 2022; Ambrosi et al., 2009; Bazzicalupi et al., 2013; Mohammad Abu-Taweel et al., 2024; Mohanasundaram et al., 2021; Singh et al., 2021, 2022). Among these, pyridine forms stable complexes by coordinating with metal ions through the nitrogen atom in its ring and exhibits selectivity towards metal atoms due to this property (Mohammad Abu-Taweel et al., 2024; Sahın, 2022). Pyridine derivatives are effectively used in the detection of metal ions in numerous applications (Bazzicalupi et al., 2009; Faridbod et al., 2015; Li et al., 2011; R. Kumar et al., 2018; Sahu et al., 2020; Yang et al., 2014). In this context, benzyloxy-substituted pyridine derivatives have been reported in the literature with respect to both their metal-binding behavior and fluorescence properties, with contributions from the benzyloxy or pyridine groups through electronic and steric effects (Antony Muthu Prabhu et al., 2010; Koçoğlu, 2024; Mahato et al., 2025)

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The nitro group acts as a strongly electron-withdrawing substituent due to its high electronegativity (Huheey, 1966). The thermal behavior of nitro-containing compounds is mainly determined by conjugation, aromaticity, and hydrogen bonds in their molecular structures (Deschamps & Parrish, 2015; Gutowski & Cudziło, 2021). The decomposition of nitro-containing compounds, which occurs with gas release during slow heating, generally begins above 300 °C, which is considered one of the fundamental indicators of the thermal resistance of these structures (Gutowski & Cudziło, 2021). Since the thermal behavior of nitro-containing compounds is critical for safety, various studies have been conducted in this area (Agrawal et al., 2000; Koçoğlu, 2024; Koçoğlu et al., 2022; Şen et al., 2020; Thangaraj et al., 2014, 2015). As observed in structurally related molecules, the presence of such substituents in benzyloxy-pyridine derivatives may influence conjugation and intramolecular interactions, with possible effects on thermal stability (Huczyński et al., 2008; Koçoğlu, 2024).

In this study, a new benzyloxy-pyridine compound was synthesized and characterized by spectroscopic methods (^{1}H-NMR, ^{13}C-NMR, FT-IR, and HRMS). Thermal behavior of the compound was investigated using TGA and DTA techniques. In addition, the metal selectivity of the compound towards different metal ions was investigated fluorometrically.

II. MATERIAL AND METHOD

A. Reagents and Instrument

All chemicals were used in their commercial form without purification. Chemical compounds and solvents were Sigma-Aldrich brand. Sodium and potassium iodide were used for metal selectivity studies and nitrate salts were used for other metals. The reaction was monitored by thin layer chromatography (TLC) during the preparation of the compound (stationary phase: Merck 60 PF-254; mobile phase: THF; UV source: 254 nm). Mass spectroscopy (HR-MS) results were obtained with Agilent Technologies 6224 TOF LC/MS in acetonitrile without column (ion mode: ESI+). For FT-IR analysis, a Schimadzu Infinity model spectrophotometer with an ATR attachment was used in the 4000-400 cm^{-1} range. ^{1}H-NMR and ^{13}C-NMR results were obtained by dissolution in DMSO-*d6* with a Bruker Avance Neo 500 MHz (standard: $SiMe_4$). Thermal analyses were performed in nitrogen atmosphere with Shimadzu DTG-60 instrument using a platinum pan. The metal selectivity of the compound was investigated spectrophotometrically by Molecular Devices, SpectraMax M5 spectrophotometer (solvent: EtOH; cuvette: quartz; excitation wavelength: 250 nm).

B. Synthesis of Compound ***L***

Potassium hydroxide (0.67 g; 12 mmol) was dissolved in 5 mL DMF with stirring. A solution of 2-hydroxy-3-nitro-5-bromopyridine (0.26 g, 1.2 mmol) in 5 mL of DMF was added dropwise. The mixture was stirred for 2 hours and monitored by TLC. After completion of the potassium salt formation, benzyloxy bromide (1.2 mmol) was slowly added to the reaction medium. The mixture was stirred overnight at room temperature. Then about 50 mL of distilled water was added, and a light orange solid was observed to precipitate. Stirring continued for a further time, and the precipitate formed was filtered and allowed to dry. The precipitate was recrystallized from acetonitrile (Figure 1)(m.p. = 135 °C; yield: %72).

Closed Formula: $C_{12}H_9BrN_2O_3$ FT-IR spectrum (cm^{-1}): 3059, 3046 (C–H_ar.), 1690 (C=N), 1593, 1456 (C=C) 1504, 1329 (NO_2 asy./sym.), 1269, 1203 (C–O–C), 714, 693 (C–Br). HRMS (ESI+) (CH_3CN, m/z): for [M+Na$^+$] calcd. for $C_{12}H_9BrN_2O_3Na$ 330.96945 (^{79}Br) and 332.96740 (^{81}Br); found: 330.96983 (^{79}Br) and 332.96806 (^{81}Br). ^{1}H-NMR spectrum (500 MHz, DMSO-d_6): δ: 8.77 (d, *J* = 2.75 Hz, 1 H), 8.77 (d, *J* = 2.75 Hz, 1 H), 7.32–7.38 (m, 5H), 5.21 (s, 2H). ^{13}C-NMR spectrum (125 MHz, DMSO-d_6): 153.04 (C1), 146.44 (C5), 141.21 (C7), 139.27 (C2), 136.16 (C9, C11), 129.15 (C2), 129.15 (C8, C12), 128.52 (C10), 94.34 (C4), 53.37 (C6).

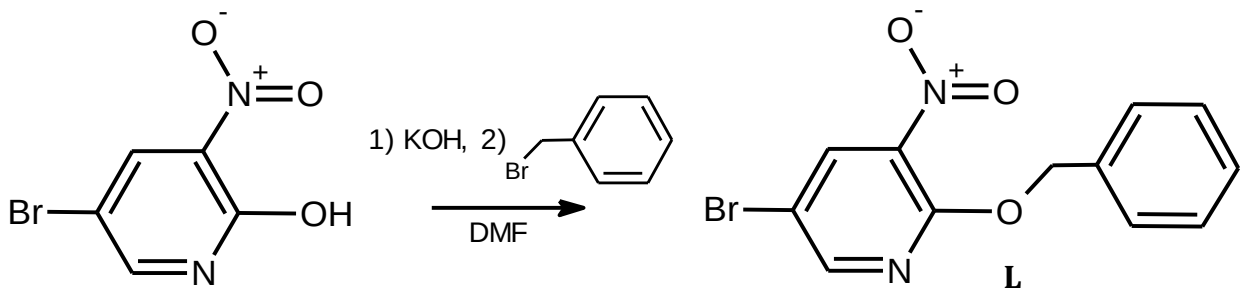


Figure 1. Synthesis of compound **L**.

III. RESULTS AND DISCUSSIONS

A. *NMR Spectra*

The NMR spectra of compound **L** were recorded in DMSO-d_6. The ^{1}H-NMR and ^{13}C-NMR spectra are presented in Figure 2, and the corresponding chemical shift values (ppm) are listed in Table 1.

Compound **L** contains nine protons. The H3 and H5 were observed to be mutually split with a coupling constant of 2.75 Hz and were given two doublets at 8.77 and 8.66 ppm, each corresponding to one proton. The aromatic protons (H8–H12) of the benzene ring have given a multiplet belonging to five protons at 7.35 ppm. Although distinguishable peaks were observed in this region, they have been treated as a multiplet due to their similar chemical shifts and long-range coupling (Figure 2a). The methylene bridge protons H6 (-O-CH2-) connecting the two aromatic rings were given a singlet at 5.21 ppm corresponding to two protons.

The compound contains twelve carbon atoms. Considering the equivalence of C8/C12 and C9/C11, ten distinct signals were expected in the ^{13}C NMR spectrum. However, only nine signals were observed, due to overlap of the C3 signal with the broadened peak at 129.15 ppm assigned to C8 and C12 (Figure 2b).

These NMR results, together with the other characterization data, confirm that compound **L** was successfully synthesized.

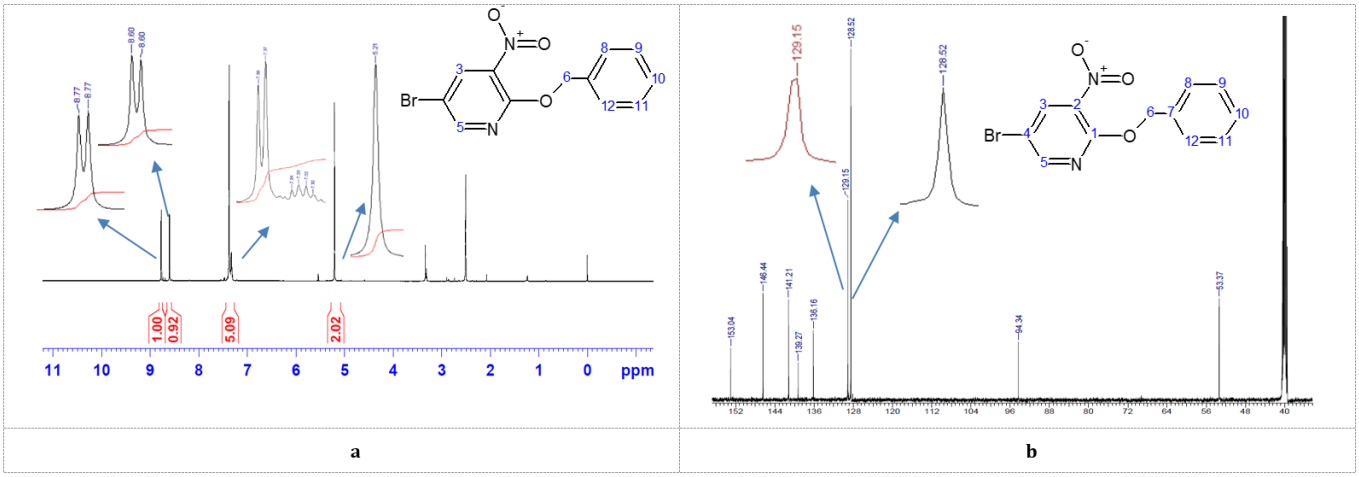


Figure 2. a)^{1}H- and b)^{13}C- NMR spectra of compound **L.**

Table 1. ^{1}H- and ^{13}C- NMR data for compound **L.**

	1	2	3	4	5	6	7	8	9	10	11	12
^{1}H-NMR			8.60 (d; 1H) $^{3}J_{5\text{-}3}$: 2.75 Hz		8.77 (d; 1H) $^{3}J_{3\text{-}5}$: 2.75Hz	5.21 (s; 2H)		7.35 (m; 5H)				
^{13}C-NMR	153.04	139.27	129.15	94.34	146.44	53.37	141.21	129.15	136.16	128.52	136.16	129.15

s: singlet; d: doublet; m: multiplet

B. *FT-IR Spectrum*

The FT-IR spectrum for compound **L** is given in Figure 3 and selected characteristic peaks are given in Table 2.

Table 1. Selected FT-IR bands for compound **L** (cm^{-1}).

Compound	ν(C=C)	ν(NO_2)	ν(C=N)$_{pyr.}$	ν(C-O-C)
L	1593;1456(m)	1504;1329(s)	1690(s)	1270(s)

m: medium; s: strong

Compound L has characteristic functional groups detectable by FT-IR, including aromatic C=C and C=N bonds, a C–Br bond, an etheric –C–O–C– bond, and a nitro group (Figure 1).

The stretching vibrations of the aromatic groups in compound **L** were observed at 3059 and 3046 cm^{-1}. The strong peak observed at 1690 cm^{-1} belongs to C=N bonds in the pyridine group (Konakanchi et al., 2022). The peaks observed at 1504 and 1329 cm^{-1} correspond to the asymmetric and symmetric stretching vibrations of the nitro group (Koçoğlu, 2024; Núñez-Quintero & Hernández-Rivera, 2006; Ramalingam et al., 2008). The C–O–C stretching vibrations were observed at 1269 and 1203 cm^{-1} (Koçoğlu et al., 2021; Muddasar et al., 2024). Additionally, C-Br stretching vibrations were detected at 714 and 693 cm^{-1} (Boopalachandran et al., 2012). These observations support the presence of the

expected functional groups in compound **L**.

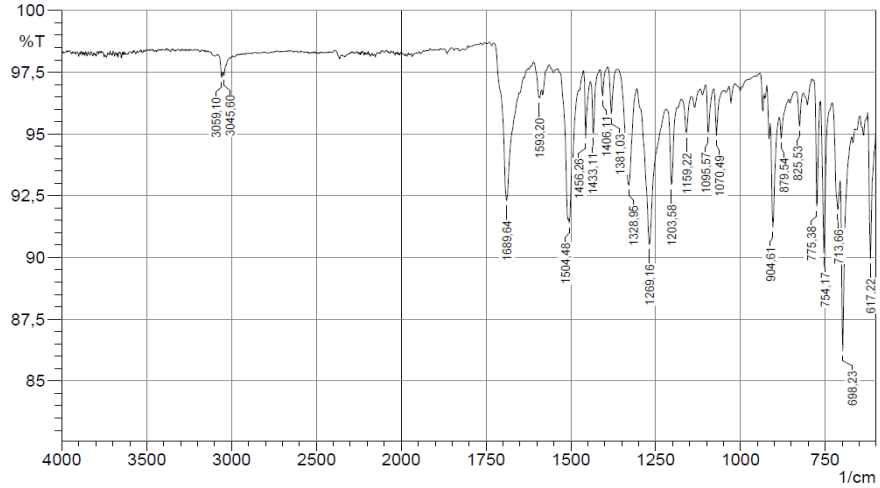


Figure 3. FT-IR spectrum of compound **L.**

C. Mass Spectrum (HRMS data)

The HRMS spectrum of the synthesized compound **L** is shown in Figure 4, and the analytical data, theoretical mass values, and margin of errors (ppm) are presented in Table 3.

The molecular formula of compound **L** is C12H9BrN2O3. The two stable natural isotopes of bromine in the structure are ^{79}Br and ^{81}Br, with natural abundances of 50.7% and 49.3%, respectively (Meija et al., 2016). Accordingly, two molecular ion peaks (m/z) were theoretically calculated as 307.97968 and 309.97763 (Scientific Instrument Services, n.d.). However, no peaks corresponding to these values were observed in the HRMS data.

Table 3. HRMS data for compound **L.**

Compound	Molecular ion	Isotopes	Mass (measured)	Mass (calculated)	Error ratio (ppm)
L	$[M+Na]^+$	^{79}Br	330.96983	330.96945	1.15
		^{81}Br	332.96806	332.96740	1.98

In the technique used, the molecular ion peak may appear as protonated and sodiated forms ($[M+H]^+$ and $[M+Na]^+$) (March et al., 2017; Kildgaard et al., 2014). Accordingly, when the obtained data were re-examined, the peaks corresponding to the $[M+Na]^+$ ions were found at 330.96983 and 332.96806 with low error ratio values (for ^{79}Br and ^{81}Br isotopes) compared to the calculated values (Figure 4) (Table 3) (Brenton & Godfrey, 2010; Scientific Instrument Services, n.d.).

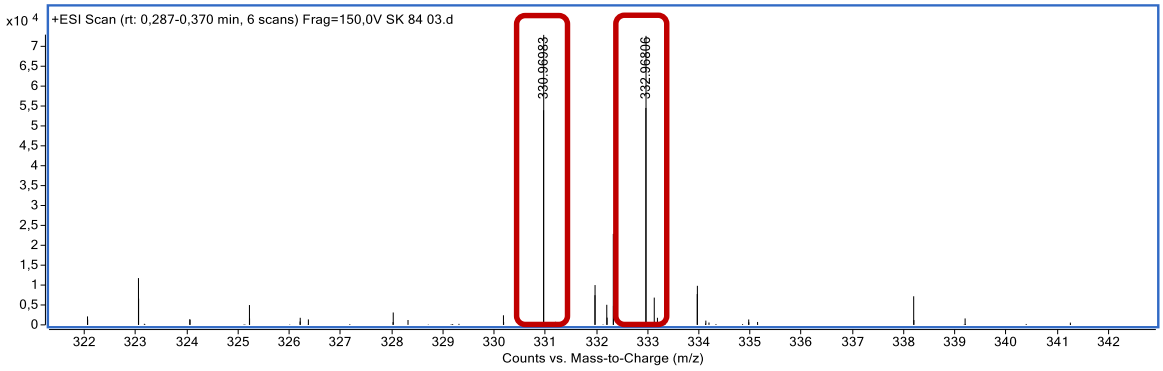


Figure 4. HRMS spectrum of compound **L.**

D. Thermal Behaviors (TGA/DTA)

TGA/DTA data on the thermal behavior of compound **L** are given in Figure 5.

The thermal behavior and decomposition of compound **L** could not be clarified according to the Ω rules due to the presence of a nitro group in its structure (Klapötke, 2015; Şen et al., 2014).

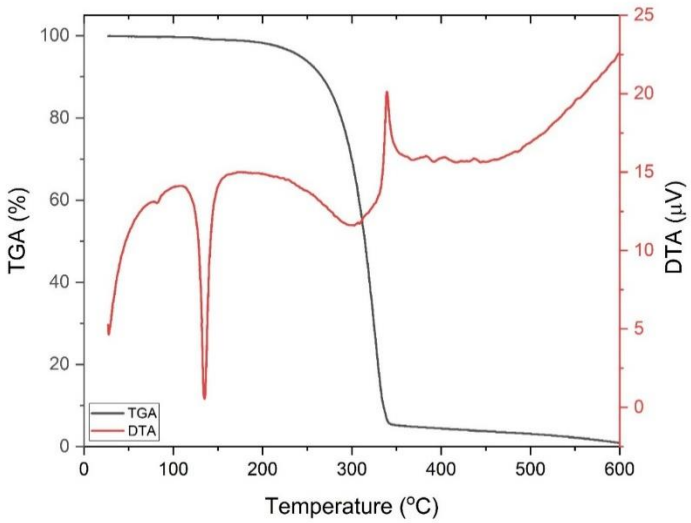


Figure 5. Thermal analysis of compound **L.**

The thermal decomposition curve of this molecule shows a strong endotherm at 135 °C. At this temperature, no mass loss is observed and there is no change in the chemical structure of the molecule. This indicates that this temperature is the melting point of compound **L**.

Decomposition began at around 300 °C. Immediately afterwards, a strong exotherm was observed at 339 °C. This indicates the breaking of the $-NO_2$ group and the C–O bond in the ether bridge between the aromatic rings (Fayet et al., 2011).

C-Br bond breakage from the aromatic ring is known to occur after 300 °C (Haynes, 2016). Thermal analysis shows that the entire mass is lost, indicating that no inorganic residue is formed and that Br is removed from the structure as HBr.

E. Metal Selectivity

The data of the metal selectivity study of compound **L** are given in Figure 6. In this context, firstly, 5×10^{-5} M solution of the compound in ethyl alcohol was prepared and mixed with the solutions of metal salts in ethyl alcohol as 1:100 (ligand:metal) ratio and kept for 24 hours.

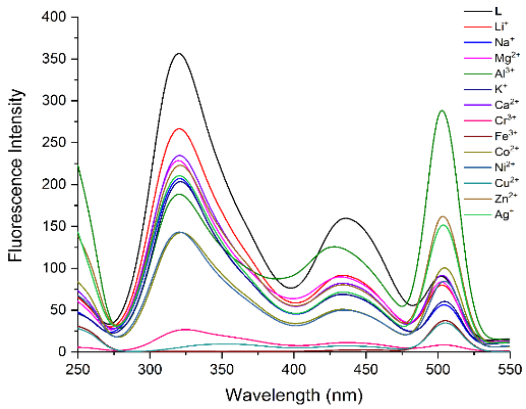


Figure 6. Metal ion selectivity of compound **L** (EtOH, quartz cuvette, λ_{ex} = 250 nm).

The solution of compound **L** excited at 250 nm gave an emission at 320 nm. The addition of metal ions did not result in a significant shift in the emission wavelength.

However, a general fluorescence quenching is observed which is much more pronounced in the presence of Cr^{3+}, Fe^{3+}, and Cu^{2+} ions (Figure 6). The absence of emission shifts combined with the decrease in intensity suggests that the quenching mechanism may primarily arise from interactions between the pyridine nitrogen atoms in compound **L** and the metal ions (Ma et al., 2021; Wang et al., 2020). In addition, Fe^{3+} and Cu^{2+} ions are paramagnetic, which may enhance non-radiative decay processes and lead to stronger fluorescence quenching (Chamlagai et al., 2026; Lakowicz, 2006). A potential contribution from photoinduced electron transfer (PET) between the pyridine moiety and the metal ions can

also be considered to account for the observed reduction in intensity (He & Liu, 2016; Sharma & Ghosh, 2021).

According to these results, it can be easily stated that compound **L** shows high metal selectivity, especially towards Cr^{3+}, Fe^{3+} and Cu^{2+}.

IV. CONCLUSION

In this study, a new ethereal compound containing benzene and pyridine rings was synthesized and characterized by spectroscopic methods. The thermal behavior and metal selectivity of the synthesized compound were also investigated.

Since the synthesized compound contains a nitro group, it was important to examine its thermal properties. In the study, it was observed that the structure remained intact until high temperatures, and the molecule disintegrated without leaving any residue above 300 °C. These findings indicate good thermal stability of compound **L**.

As expected in the metal selectivity studies of the compound containing the pyridine ring, a fluorescence quenching effect was observed, especially with Cu^{2+} and Fe^{3+}. With further studies, these properties can be investigated in more detail by spectrophotometric titration at different pH values, temperatures, wavelengths and metal ions for which the compound shows selectivity.

These findings suggest that compound **L** is a thermally stable, pyridine-based small molecule that exhibits selective fluorescence in response to specific metal ions. This highlights its potential as a functional structure for further research.

The biological and pharmaceutical properties of compound **L** were not examined in this study; however, its small molecular size and related examples in the literature suggest that it is suitable for future ADME and biological investigations.

DECLARATIONS

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Author Contributions: All parts of the study were conducted by the Author.

Conflict of Interest: The author declares no conflict of interest.

Supporting Institutions: This research received no external funding.

Ethical Approva: This study does not involve human or animal participants. All procedures followed scientific and ethical principles, and all referenced studies are appropriately cited.

Plagiarism Statement: This article has been evaluated for plagiarism, and no instances of plagiarism were detected.

Use of AI Tools: The author declares that no Artificial Intelligence (AI) tools were used in the creation of this article.

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