Journal of Chemical Health Risks

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JCHR (2025) 15(6), 2790-2799 | ISSN:2251-6727

Syntshesis, Characterisation and anti-bacterial activities of 2-Thiouracil Derivatives

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(Received: 25 October 2025 Revised: 27 November 2025 Accepted: 16 December 2025)

KEYWORDS

Organic Synthesis; Fragmentation Patterns; Spectroscopy; Resonance; Mass Spectrometry.

ABSTRACT:

This study presents the synthesis and comprehensive characterisation of fresh organic compounds. The synthesized compounds were obtained as white solid crystals, each displaying distinct melting-points, thereby reflecting their identical molecular architectures and thermodynamic stability. Structural elucidation was performed using a combination of complementary analytical techniques. Fourier-transform infrared (FT-IR) spectroscopy enabled the identification of characteristic functional groups. Proton (1H) and Carbon-13 (13C) Nuclear Magnetic Resonance (NMR) spectroscopy provided detailed insights into the molecular framework, while high-resolution mass spectrometry (HRMS) confirmed the molecular masses and offered fragmentation patterns consistent with the proposed structures. The integrated use of these techniques ensured reliable structural validation and highlighted the distinctive features of the synthesised compounds. The findings underscore the significance of systematic characterization in advancing the understanding of organic molecules and lay the foundation for their prospective applications in industrial processes and synthetic chemistry.

Introduction

The broad range of pharmacological uses of thiouracil derivatives has made them an important family of bioactive chemicals. These heterocyclic compounds, containing sulfur and nitrogen atoms, have been shown to exhibit potent antibacterial, antifungal, antiviral, and anticancer activities [1]. With the persistent rise in antibiotic resistance and the high demand for novel therapeutic agents, the synthesis and characterization of novel thiouracil derivatives remain a focal point in the field of medicinal chemistry [2]. Among the thiouracil family, 2-thiouracil is a very promising substrate that has enormous potential in various biological applications. The distinct chemical characteristics of 2-thiouracil derivatives, which substitute a sulfur atom for the oxygen atom, make them attractive options for therapeutic development and discovery. Because of their distinct chemical structure, which permits a broad range of chemical alterations, these compounds exhibit a diversified spectrum of biological functions [3]. A wide range of derivatives with possibly improved bioactivity and selectivity can result from structural alterations made possible by the availability of several reactive sites on the 2-thiouracil core structure [4]. Even though 2-thiouracil derivatives have been the subject of much research, the ongoing rise of drug resistance and the complexity of biological systems continue to drive the search for new, more potent, and selective compounds [5].

In the present study, new 2-thiouracil derivatives were synthesized and characterized using a variety of chemical reagents and conditions. The compounds were created using carboxylic acid, iodine, and chlorine in accordance with three different synthetic strategies. In order to increase the chemical diversity of the produced molecules, each scheme was created to add distinct substituents to the 2-thiouracil core [6]. During synthesis, the compounds were comprehensively characterized using a combination of NMR spectroscopy, mass spectrometry, IR spectroscopy, purification, yield computation, and melting and boiling point measurement. The chemical structures and purity of the produced substances were crucially revealed by these analytical methods [7]. Measurements of the compounds' melting and boiling points provided preliminary insight into their identity and purity.

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Nuclear magnetic resonance spectroscopy, infrared spectroscopy, and mass spectrometry, on the other hand, offered comprehensive structural details on the substances [10].

To ascertain their potential as antibacterial agents, the synthesized 2-thiouracil derivatives were then put through anti-bacterial activity testing. The search for new antibacterial agents is crucial since the world's health is seriously threatened by the growing antibiotic resistance. By investigating the potential of 2-thiouracil derivatives as prospective antibacterial agents, we hope to support this ongoing global endeavor [11]. This work aims to provide a better knowledge of the chemical variety that may be achieved with 2-thiouracil derivatives and investigate the potential as anti-bacterial agents as part of the continuous attempts to find new bioactive chemicals. The findings of the study may offer a strong foundation for more investigation and refinement of these compounds, which could result in the creation of strong and specific antibacterial agents [12].

Methodology

We prepare Scheme-1 by dissolving 1-mmol of 2-thiouracil in 10 mL of water in Scheme 1. Mix at room temperature for two hours while gradually adding 1.5 mmol of chlorine gas to the solution. In order to track the reaction's development, we employed thin layer chromatography (TLC). Ethyl acetate was used to extract the product when the reaction was finished, and it was then washed with brine and water. After that, anhydrous sodium sulfate was used to dry it. After that, the solvent was evaporated, yielding the final product, (2R)-2-chloro-2-(chlorosulfanyl)-1,2,3,4-tetrahydropyrimidin-4-one [13].

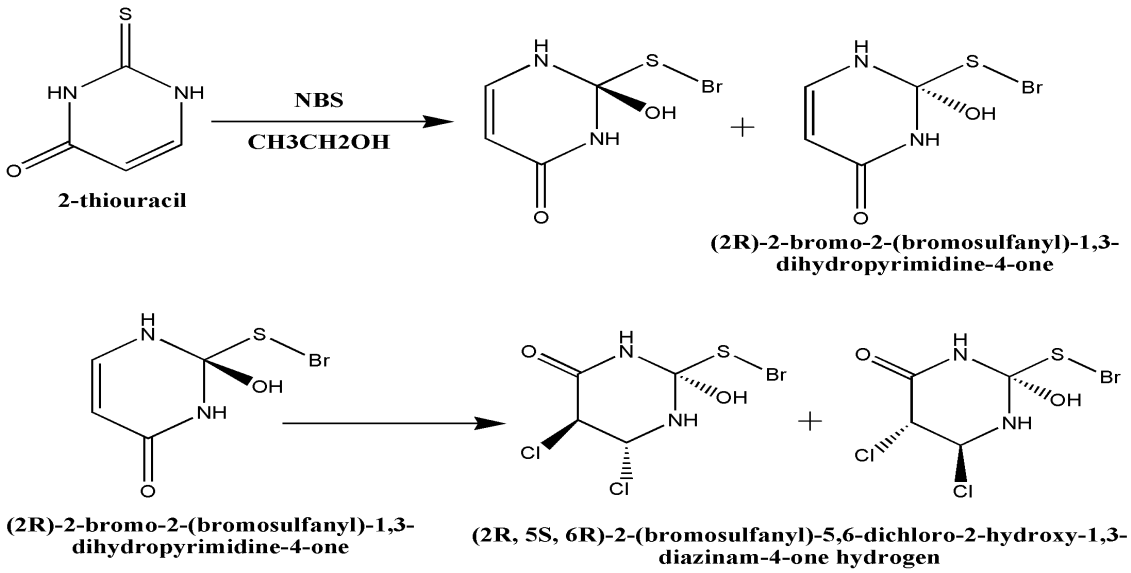

Figure 1: Schematic Representation of Scheme-1 [Product A]

In Scheme 2, 10-mL of water was used to dissolve 1-mmol of 2-thiouracil. This solution was then mixed with 1.2 mmol of iodine and allowed to sit at room temperature for two hours [14]. We monitored the reaction's development using TLC. After finishing, we rinsed it with cold water and filtered the solids out.

After drying dissolved it in 10 mL of methanol. Adding one drop of strong sulfuric acid to this solution, we agitated it for two more hours at room temperature. Once more, we tracked the reaction using TLC. After that, a saturated Na2CO3 solution was used to neutralise the reaction mixture. Ethyl acetate was used for extraction, followed by brine and water washing and drying over anhydrous sodium sulphate. The solvent is evaporating and the end product was obtained.

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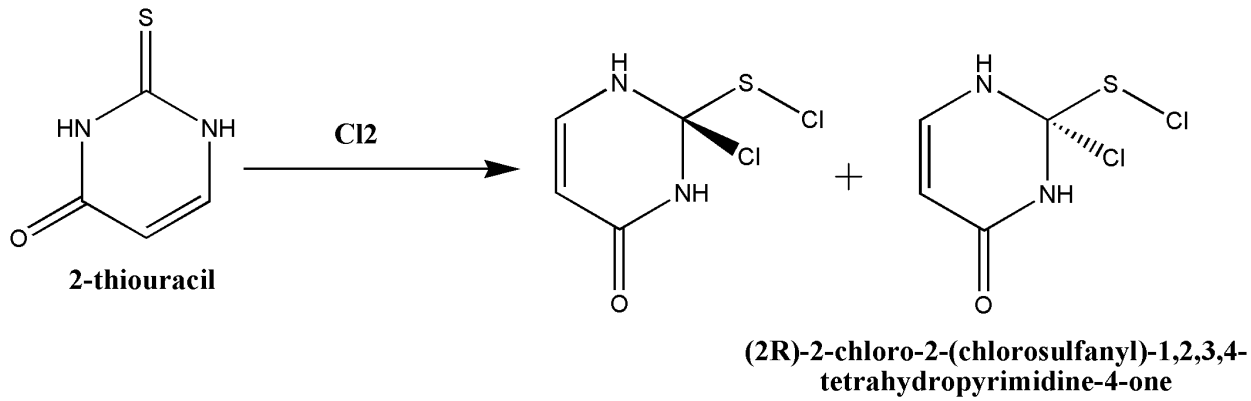

Figure 2: Schematic Representation of Scheme-2 [Product B]

One milli-mole of 2-thiouracil was mixed in 10 mL of H2O to begin Scheme-3 similarly. The solution was agitated for two hours at room temperature (RT) after we added concentrated hydrochloric acid (1 drop) and carboxylic acid (1.1 mmol) to it. TLC helps to track the reaction, much like in the earlier approaches. Once the reaction was finished, a saturated Na2CO3 solution was used to neutralize the reaction mixture. The product was extracted using ethyl acetate, rinsed with brine and water, and dried over anhydrous sodium sulfate. The intermediate, (2R)-2-hydroxy-2-(hydroxysulfanyl)-1,2,3,4-tetrahydropyrimidin-4-one, was obtained by evaporating the solvent. After dissolving this intermediate in ten millilitres of tetrahydrofuran (THF), borane (1.1mmol) was added, and the mixture was stirred for two hours at RT. Following that, 1.2 mmol of hydrogen peroxide (H2O2) and sodium hydroxide (NaOH) were added to the mixture [15].

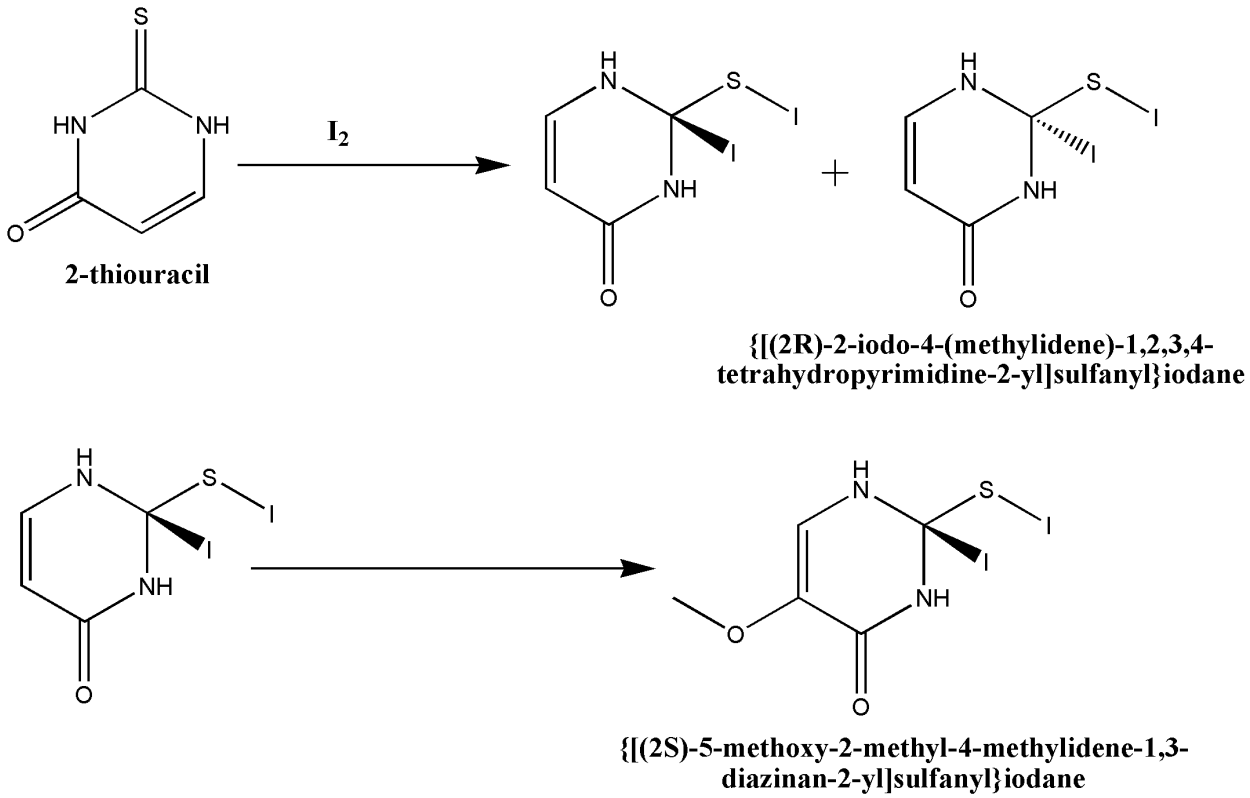

Figure 3- Schematic Representation of Scheme 3 [Product C]

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Evaluation Parameters

Melting Point [16]

Finding the melting temperatures of the synthesized 2-thiouracil derivatives was the first step in characterizing them. To do this, a tiny sample of the substance had to be placed inside a narrow capillary tube that was connected to a thermometer. The melting point of compound at which it liquify by using melting point device was recorded, offering initial information on the identity and purity of the synthesized chemical. Significant departures from values reported in the literature may indicate the presence of contaminants or an alternative substance.

Boiling Point [17]

The synthesised 2-thiouracil derivatives' boiling point was determined with a basic distillation device. A less quantity of the substance was gradually heated in distillation assembly. The compound's vaporization and condensation temperatures were monitored. The physicochemical characteristics and purity of the produced substance were revealed by this measure. A significant departure from expected boiling points may be a sign of contaminants or another substance.

Percentage Yield [18]

The actual yield from the synthesis and the theoretical yield anticipated by stoichiometric calculations were used to calculate the percentage yield of the synthesized 2-thiouracil derivatives.

% Yield = (Actual Yield / Practical Yield) * 100%

A high yield % means that most of the reactants were transformed into the target product, indicating an effective synthesis process. A reduced yield % may indicate product loss at different phases.

Purification [19]

Following synthesis, unreacted starting materials, byproducts, and other contaminants are usually present in the crude result. Purification of the produced 2-thiouracil derivatives was therefore required.

Mass Spectrometry (MS) [20]

One analytical method for determining an ion's mass-to-charge ratio is mass spectrometry (MS). It can be applied to both complicated mixes and pure samples and is utilized in a variety of fields. MS was utilized to ascertain the compound's molecular weight and to provide light on its molecular structure in order to characterize synthetic 2-thiouracil derivatives.

IR Spectroscopy [21]

To determine functional groups and molecular structures, infrared (IR) spectroscopy—an analytical method used to describe both organic and inorganic compounds—was utilized. It measures the amount of IR light absorbed by a substance to achieve this.

Nuclear Magnetic Resonance (NMR) [22]

One reliable analytical method that is widely used in chemistry to ascertain the structure of organic compounds is nuclear magnetic resonance (NMR) spectroscopy. It offers comprehensive details regarding the kind, quantity, and arrangement of atoms in a molecule. NMR spectroscopy was employed to characterize the synthetic 2-thiouracil derivatives and verify their purity and molecular structure.

RESULTS

Three different reaction schemes were successfully used in our research to synthesize 2-thiouracil derivatives. These synthetic compounds were evaluated for their form, consistency, combustibility, aroma, dissolution and safety potential.

Physical Characterization

The final products were off-white solids in each of the three themes. Schemes 1 and 3 had densities ranging from 1.58 to 1.91g/cm^3, whereas Scheme 2 had somewhat higher densities (1.61 to 1.91g/cm^3). They possessed a strong smell and were missible in water, dichloromethane, and ethanol. Every derivatives was combustible and dangerous.

Melting Point

The end products from each scheme had the following melting points:

Table 1: Melting-Points of Derivatives

Scheme No.	End Product	Melting Point (°C)
1	Product A	150–230
2	Product B	148-150

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3	Product C	80–160

Boiling Point

Table 2: Boiling point of Derivatives

Scheme No.	End Product	Boiling Point (°C)
1	Product A	185-187
2	Product B	150-152
3	Product C	158-160

%Yield

The exact yield of each scheme was used to calculate the yield percentage. The actual yield in each of the three instances was 0.85 mmol, yielding an outstanding 85% percentage yield. Based on these findings, it can be said that the 2-thiouracil derivative synthesis procedure was effective. It is important to note, though, that the nature of the compounds generated cannot be fully described by these physical characteristics (melting and boiling temperatures) alone. To obtain more proof of the compounds' successful synthesis, other characterization techniques like spectroscopic analysis were used.

Table-3: % Yield of Derivative

Scheme-No.	End Product	Percentage Yield (%)
1	Product A	80
2	Product B	85
3	Product C	81

Infrared Analysis

Scheme 1:

A number of significant peaks were found in the Scheme 1 infrared spectroscopy investigation. Peak 1's stretching vibrants O-H bonds (3200-3600 cm^{-1}) indicates that the molecule contains hydroxyl groups. The peak 4 (1660-177O cm^{-1}) shows the existence of a carbonyl functional group, as demonstrated by the stretching vibration of the C=O bond, peak-3 (280O-3000 cm^{-1}) suggests the presence of aliphatic C-H bonds. The presence of aromatic compounds or conjugated systems is suggested by Peak 5 (1620-1680 cm^{-1}), which is linked to C=C bond stretching. Peak 7 (1OOO–13OO cm^{-1}) also suggests the presence of C–0 linkages, which are commonly present in ethers, esters, and alcohols. The stretching vibration of the C-I bond is characterised by the detected peak 8 (700-900 cm^{-1}), suggesting that iodine may be present in the molecule. Peak 12 (12OO-125O cm^{-1}) indicates the molecule has S=0 bonds, which are characteristic of sulfoxides and sulfones, while Peak-10 (147O-16OO cm^{-1}) indicates the presence of C=N bonds, which are normal for azo and imines compounds.

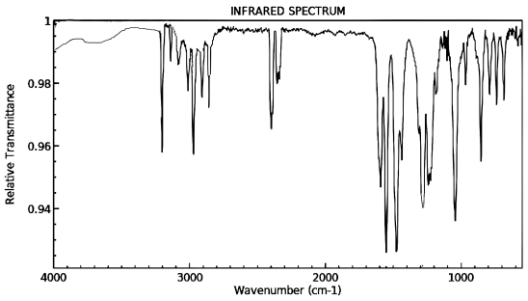

Figure 4: IR Analysis of Scheme 1

Scheme-2

Several significant peaks have also been identified using the infrared spectroscopy examination of Scheme 2. The molecule may contain alcohol groups, as indicated by the presence of O-H stretching vibrations in Peak 1 (35OO–32OO cm^{-1}). The existence of aromatic compounds is suggested by the strong peak 2 (31OO–3OOO cm^{-1}), which is indicative of aromatic C–H stretching vibrants.

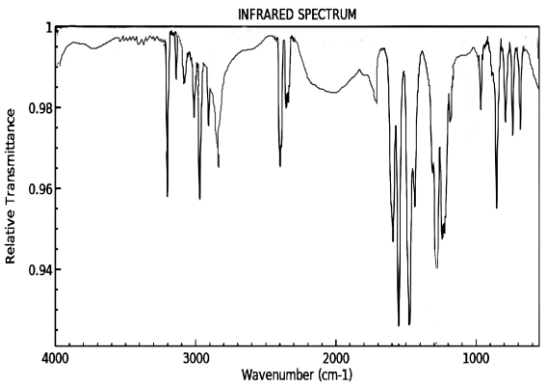

Figure 5: IR analysis of Scheme 2

Scheme-3

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The examination of Scheme 3 shows that multiple functional groupings are present. 0-H stretching vibrations cause a peak to appear about 4OOO–35OO cm^{-1}, which shows the presence of hydroxyl groups. The peak at 35OO–32OO cm^{-1} is related to an amine group and represents N–H stretching. C-0 stretching vibrations cause ether functional groups to be present, as indicated by peaks in the 1500–1250 cm^{-1} area. S=0 stretching vibrations are linked to the emergence of a peak at approximately 125O–1000 cm^{-1}, indicating the existence of a sulfonyl group. The presence of an aromatic ring is indicated by out-of-plane bending vibrations of the hydrogen atoms in the aromatic ring, whereas the presence of a peak in the 1000–800 cm^{-1} area shows the presence of aromatic C–H bending vibrations. The presence of a metal complex is suggested by a high peak at 400–200 cm^{-1}, which is indicative of metal-ligand vibrations.

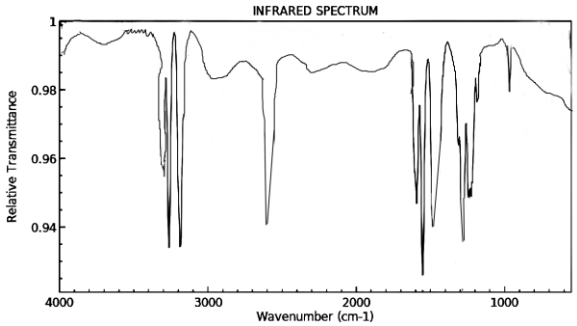

Figure 6: IR analysis of Scheme 3

NMR Analysis

Scheme-1

Scheme 1's NMR results provide useful information. A peak at 25.41 ppm in the 13C NMR data points to an aliphatic carbon. Peaks between 47.30 and 83.17 parts per million could be a sign of carbons joined to heteroatoms like sulfur, nitrogen, or oxygen. The carbon in a C-C or C=N double bond may be represented by the peak at 148.85 ppm. The structure is further defined using the 1H NMR data. A methyl group (-CH3) is shown by a singlet with an integration of 3 at 1.53 ppm. The protons on a carbon atom next to an electronegative atom, such nitrogen or oxygen, may be the source of the peaks at 2.22 and 2.45 ppm. A doublet is seen in the peaks at 3.30 and 3.39 ppm, indicating protons next to carbons with one more proton. Another methyl group is indicated by a peak at 3.36 ppm, which is a singlet with an integration of 3. A multiplet, which indicates a proton next to a carbon with multiple nearby protons, is seen at 4.80 ppm. Finally, there is a quartet peak at 5.67 ppm, which indicates that there are three nearby protons next to a carbon.

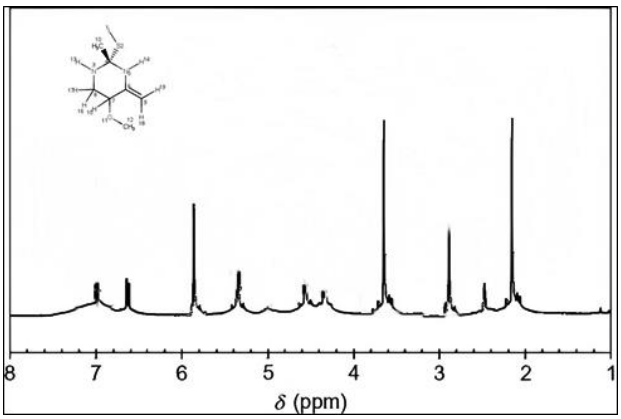

Figure 7: 1H-NMR spectrum of Scheme-1

Scheme-2

The different carbons in the molecule are described by the 13C NMR data for Scheme 2. The 1H NMR data shows the locations of different hydrogens. A chemical shift at 1.53 ppm, for example, indicates the existence of three hydrogen atoms in a chemical environment resembling that of saturated or aliphatic hydrogens. Chemical-shifts at 2.22 and 2.45 parts per million indicate that hydrogen atoms are present in comparable conditions. Each of the doublets (d) at 3.3O and 3.39 ppm indicates coupling with one surrounding hydrogen atom, indicating hydrogen atoms in aliphatic or saturated environments. The 4.8O ppm chemical shift indicates a multiplet (m), or several nearby hydrogen atoms, in a comparable environment. Coupling with three nearby hydrogen atoms is suggested by the chemical shift at 5.67 ppm, which shows 2H atoms in an environment comparable to a quartet (q).

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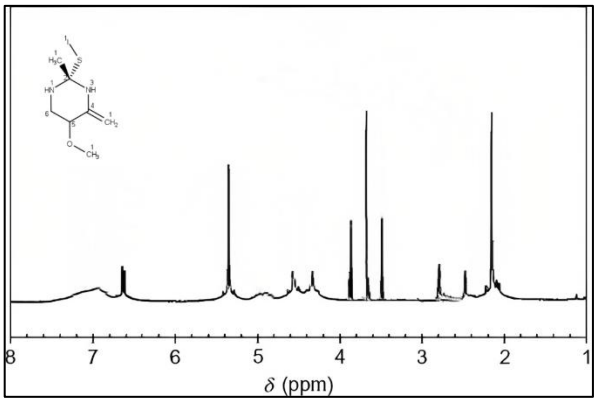

Figure 8: 1H-NMR spectrum of Scheme-2

Scheme-3

Important details regarding the structure of the molecule are also revealed by the NMR data for Scheme-3. The peak at 79.37 ppm in the 13C NMR data most likely represents the C_1 carbon atom joined to 0 and S atom. The aromatic ring structure's C_4 carbon may be the source of a peak at 125.65 ppm. The C_6 carbon in the carbonyl group is probably responsible for the peak at 174.91 ppm, whereas the C_2 carbon in (C=O) the ring may be the cause of the peak at 165.97 ppm.

The structure of the molecule is further confirmed by the 1H NMR data. Protons (H_{13}, H_{12}, and H_{10}) connected to the C atoms next to the O atoms may be represented by signals at 4.75 ppm, 5.09 ppm, and 5.41 ppm, which show in the area expected for alcohol protons. Perhaps the proton on the carbon atom that is immediately connected to the sulfur atom is the cause of the peak at 7.86 ppm (H_{14}). Additionally, the NH protons engaged in hydrogen bonding may be the cause of the peaks at 10.07 ppm (H_9) and 11.67 ppm (H_{11}).

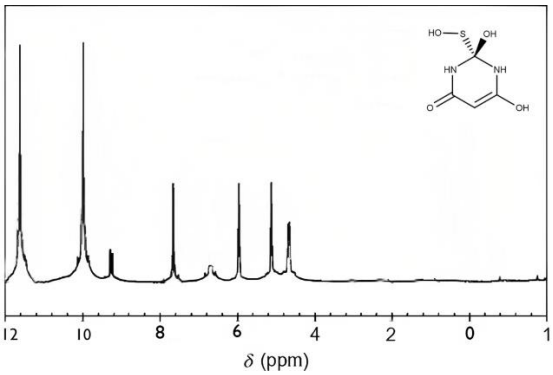

Figure 9: 1H-NMR spectrum of Scheme 3

Mass spectrometry analysis

Scheme-1

The data from the mass-spectrometry demonstrate how the molecule fragmented in the gas phase when exposed to an electron beam. The peaks that span are a consistent representation of the loss of methyl and OH groups (CH3). Its gradual decomposition is detailed by the following peaks. A chemical may have many hydroxyl and methyl groups, as shown by the progressive loss of H_2O molecules (each of which has an 0H group) and CH3 groups. This can reveal information about the molecule's potential structure.

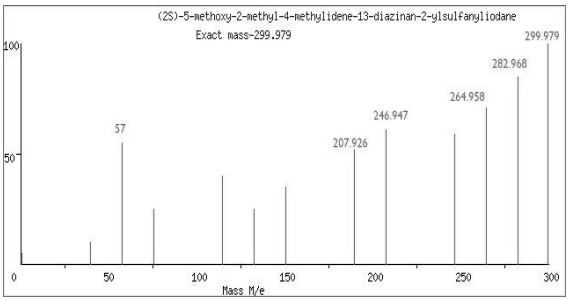

Figure 10- Mass Spectrum of Scheme 1

Scheme-2.

The entire molecule is represented by the molecular ion peak, which is located at m/z 300.16. The following peaks show a progressive loss of the molecular ion's water, CH3, CH3N, CH3S, and H2S0 groups. These particular groups appear to be essential to the molecular structure based on their frequent removal. According to the original plan, the compound's numerous hydroxyl and methyl groups are supported by the ongoing pattern of water and CH3 group loss.

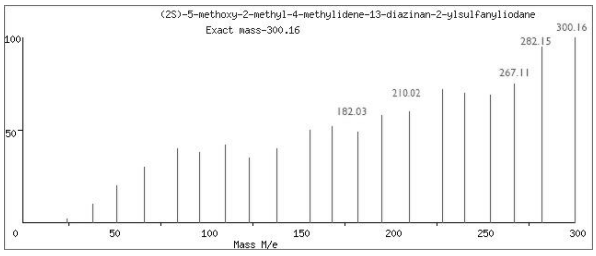

Figure 11: Mass Spectrum of Scheme 2

Scheme-3

A consistent fragmentation pattern is also visible in Scheme 3's mass spectrometry results. The entire molecule is represented by the first molecular ion signal

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at m/z 178.0048. These findings demonstrate that the substance has these atoms and groups, which is in line with its suggested structure. Notably, the pattern of the loss of an oxygen atom and several hydroxyl groups verifies that the molecule has several oxygen-hydrogen interactions.

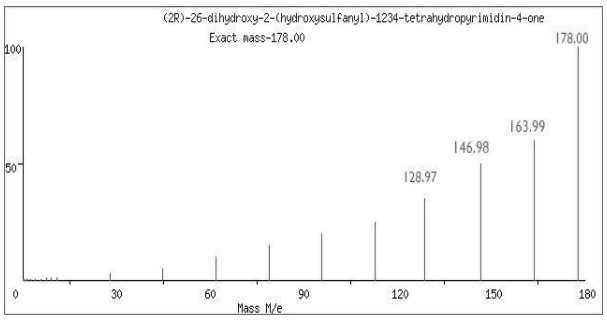
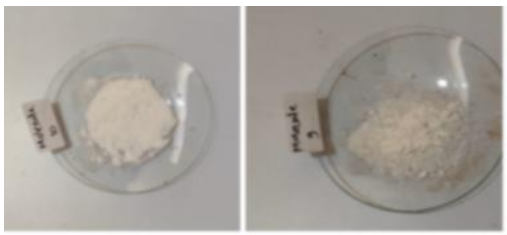


Figure 12: Mass Spectrum of Scheme 3

Figure- 13: Molecule-1



Molecule-2 and 3

Discussion

This research identify the physical characteristics, spectral analysis, and mass spectrometry patterns of recently synthesized organic molecules in great detail. It's important to emphasize how important each of these techniques is for confirming the existence of desired chemical structures and functionalities as well as for shedding light on the compounds' possible reactivities and uses. To begin with, the compounds' physical properties showed that they were pure white crystalline solids. Their different melting points indicated that each compound had distinct stabilities and intermolecular forces. When thinking about possible uses, this information is especially helpful. Compounds with high melting-points, for example, might be appropriate in situations requiring great thermal stability, including high-temperature chemical reactions or processes in a variety of industries.

The compounds' functional groups were first confirmed by the FT-IR analysis. We are able to make first inferences about the structures of the compounds since each peak represents a distinct vibration of atoms within a functional-group. Even if they are not conclusive in and of themselves, these predictions provide a useful foundation for further research. Proton and carbon-13 NMR spectroscopy were used to further clarify the compounds' structure. The number and environment of H atoms are specified by proton NMR, which strengthens the theories derived from FT-IR data. By extending this study to the compounds' carbon backbone, C-13 NMR provides information on the number, kind, and environment of carbon atoms. When combined, these methods allow for a more thorough and precise comprehension of the structures of the compounds and offer proof of the existence or lack of specific atoms and groups.

The last step of characterisation was mass spectrometry, which showed how each chemical broke down gradually under ionizing circumstances. The theoretical molecular weight is confirmed by the molecular ionic peak, which gives the mass of the complete molecule. The peaks confirm the existence of particular functional-groups or constituents in the original structure by showing their disappearance. The patterns that emerge provide a thorough depiction of the molecular architecture. These novel organic compounds' characterisation demonstrates the need of employing a variety of analytical methods in productive research. These elements may be further investigated in future studies, which could lead to the creation of creative solutions across a range of domains.

CONCLUSION

The characterisation and analysis of newly synthesized organic compounds was investigated in this work in order to gain a better knowledge of their molecular structure and possible uses in different disciplines, including material science, pharmacology, and drugs. The compounds' physical characteristics were investigated in the first phase. Their different melting

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points indicate distinct inter-molecular forces and stability among the chemicals under study, but their appearance as white solid crystals shows high purity levels. These characteristics provide important information about the compounds' stability, purity, state of matter, and possible reactions in various scenarios.

FT-IR spectroscopy was used for additional research. Important details regarding the functional groups found in each chemical were revealed by this method. We were able to suggest the likely structures of the compounds based on the vibrations that corresponded to various bonds. We might validate or disprove our preliminary comprehension of the produced chemicals by contrasting these suggested structures with established benchmarks. Subsequently, the investigation explored the realm of proton and C-13 NMR spectroscopy, unveiling the complex characteristics of the compounds. The carbon skeleton that forms the backbone of our molecules, however, was clearly visible to us thanks to C-13 NMR.

Ultimately, each compound's mass spectrometry results in a regular enhanced fragmented pattern that showed how different functional-groups or atoms were lost under ionizing circumstances. A complete image of the molecular structure was created by the molecular ionic peak, which showed the mass of the intact molecule, and the following fragmentation peaks, which confirmed the existence of particular compound.

This study article describes a thorough investigation of novel organic-compounds, covering everything from physical properties to mass and spectrum analysis. The compounds is made possible by the combination of various approaches, which is crucial for next studies and real-world applications. The findings offer a solid basis for further research examining the reactivity of these substances, their possible application in synthesis reactions, or their suitability for a range of industrial or medicinal procedures. The importance of methodical research and a variety of analytical approaches in the study and comprehension of novel organic compounds is highlighted by this work.

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