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Eco-Friendly Synthesis of a Coumarin-Containing Methylsulfanyl Pyran Derivative: A Green Chemistry Perspective

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Abstract
Green chemistry provides an effective approach for developing synthetic methodologies that minimize the use of hazardous substances, reduce energy consumption, and promote more sustainable chemical processes. In the present study, a green-chemistry-oriented synthesis of 4-methylsulfanyl-2-oxo-6-(2-oxo-2H-chromen-3-yl)-2H-pyran-3-carbonitrile was successfully carried out through the reaction of 3-acetylchromen-2-one with ethyl 2-cyano-3,3-bis(methylthio)acrylate. The reaction was performed in ethanol using potassium carbonate (K_2CO_3) as a base at room temperature for 4 h, providing the desired coumarin-containing methylsulfanyl pyran derivative in 70% isolated yield. The synthesized compound exhibited a melting point of 70 °C and was characterized by FTIR spectroscopy. The proposed synthetic protocol incorporates important green chemistry features, including the use of ethanol as a relatively environmentally preferable solvent, a mild inorganic base, ambient-temperature reaction conditions, and a straightforward synthetic procedure. The FTIR spectral data obtained experimentally support the formation of the desired functional groups in the synthesized product. Overall, the study demonstrates a simple and practical green-oriented approach for the synthesis of a structurally complex coumarin-containing pyran derivative.

***Keywords**: Green chemistry; coumarin; pyran-2-one; methylsulfanyl; cyano compound; ethanol; potassium carbonate; FTIR; sustainable synthesis.*

Introduction

Green chemistry aims to prevent waste and reduce the use and generation of hazardous substances through the design of chemical products and processes. The twelve principles emphasize waste prevention, atom economy, safer synthesis, safer solvents and auxiliaries, energy efficiency, catalysis, and related approaches to sustainable chemical manufacture (Anastas & Warner, 1998; American Chemical Society [ACS], 2026). Reaction yield alone is not a sufficient measure of the environmental performance of a synthesis. Solvent consumption, reagent stoichiometry, purification materials, energy requirements, and waste generation can substantially influence the overall process profile. Quantitative measures such as atom economy, process mass intensity (PMI), and E-factor are therefore useful complements to isolated yield when the required mass-balance information is available (Constable et al., 2018). Coumarins are versatile oxygen-containing heterocycles with extensive synthetic and medicinal-chemistry interest. Their functionalization provides access to structurally diverse compounds, while pyran-2-one frameworks offer additional opportunities for conjugation and further chemical modification (Medina et al., 2015; Citarella et al., 2024). In the present work, 3-acetylchromen-2-one was reacted with ethyl 2-cyano-3,3-bis(methylthio)acrylate using ethanol and K_2CO_3 at room temperature. The product, 4-methylsulfanyl-2-oxo-6-(2-oxo-2H-chromen-3-yl)-2H-pyran-3-carbonitrile, was obtained in 70% yield. The work is discussed specifically from a greener-synthesis perspective, with attention to solvent selection, energy demand, waste prevention, and characterization.

2. Materials and Methods

2.1 General Synthetic Procedure

A mixture of 3-acetylchromen-2-one (0.01 M) and ethyl 2-cyano-3,3-bis(methylthio)acrylate (0.01 M) was taken in ethanol. Potassium carbonate (K_2CO_3) was added as the base. The reaction mixture was stirred at room temperature for 4 h. After completion, the reaction mixture

was subjected to the appropriate work-up and purification procedure. The isolated product was identified as 4-methylsulfanyl-2-oxo-6-(2-oxo-2H-chromen-3-yl)-2H-pyran-3-carbonitrile and was obtained in 70% yield with a reported melting point of 70 °C. fig 1 shows reaction scheme

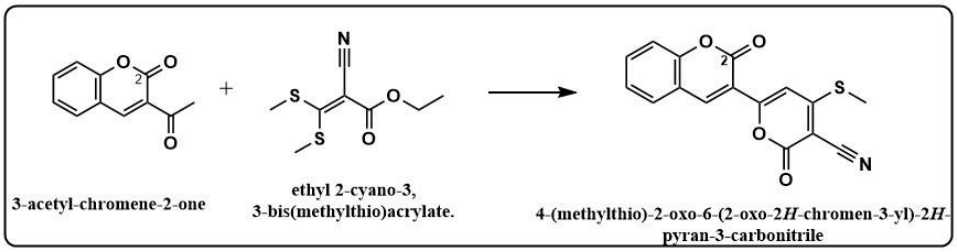


Figure 1. Reaction Scheme

3. Result and discussion

3.1 FTIR Characterization

The synthesized 4-methylsulfanyl-2-oxo-6-(2-oxo-2H-chromen-3-yl)-2H-pyran-3-carbonitrile was characterized by FTIR spectroscopy. Figure 2 FTIR spectrum exhibited characteristic absorption bands corresponding to the major functional groups present in the proposed structure. The absorption in the region of approximately **2180–2220 cm⁻¹** was attributed to the **C≡N stretching vibration**, confirming the presence of the nitrile functionality. Bands in the **carbonyl region (~1650–1750 cm⁻¹)** were assigned to the carbonyl groups of the conjugated lactone systems.

The absorptions around **1605 and 1519 cm⁻¹** were attributed to aromatic and conjugated C=C vibrations. Bands in the **1200–1000 cm⁻¹** region were associated mainly with C–O–C/C–O stretching vibrations, while the lower-frequency absorptions in the **900–700 cm⁻¹** region were assigned to aromatic C–H out-of-plane vibrations. The observed spectral features are consistent with the proposed structure of the synthesized coumarin-containing methylsulfanyl pyran derivative.

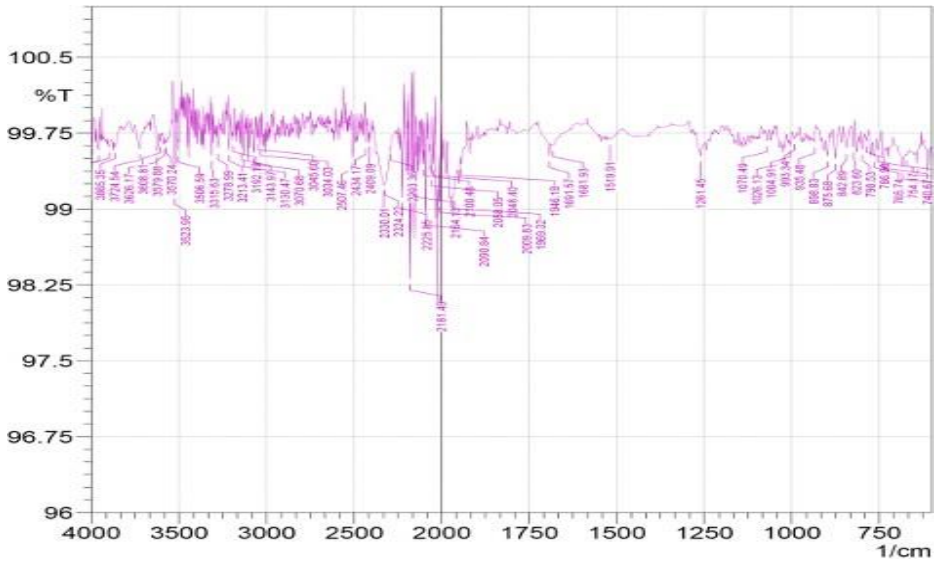


Figure 2: FTIR spectrum

3.2 Mass Spectral Analysis

The mass spectrum of the synthesized compound showed a molecular ion peak at **m/z 311.02523 (100%)**, which is in excellent agreement with the calculated exact mass of **311.0252** for the molecular formula **$C_{16}H_9NO_4S$**. The observed **M+1 peak at m/z 312.02858 (17.3%)** is consistent with the presence of 16 carbon atoms and the corresponding contribution from naturally occurring ^13C.

The **M+2 peak at m/z 313.02102 (4.5%)** is consistent with the natural isotopic abundance of ^34S, supporting the presence of one sulfur atom in the molecule. The observed isotope

distribution therefore provides strong evidence for the proposed molecular formula and supports the formation of the **4-methylsulfanyl-2-oxo-6-(2-oxo-2H-chromen-3-yl)-2H-pyran-3-carbonitrile** derivative.

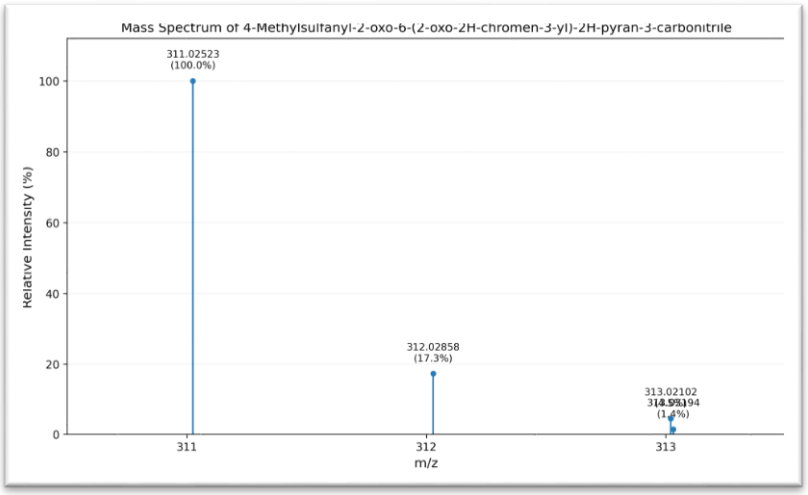


Figure: 3 Mass spectrum

4. Conclusion

A green-chemistry-oriented synthesis of 4-methylsulfanyl-2-oxo-6-(2-oxo-2H-chromen-3-yl)-2H-pyran-3-carbonitrile was achieved from 3-acetylchromen-2-one and ethyl 2-cyano-3,3-bis(methylthio)acrylate using ethanol and K_2CO_3 at room temperature for 4 h. The product was obtained in 70% yield with a melting point of 70 °C. The experimentally supplied FTIR spectrum supports the presence of important functional-group regions, including carbonyl, cyano, aromatic/conjugated, and C–O-related absorptions. The use of ethanol and room-temperature operation provides meaningful greener features, while complete green-metric validation requires additional mass-balance and waste data.

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