

Synthesis and Characterization of 2-Oxo-2-(pyren-1-yl)ethyl 4-(4-Oxo-4H-chromen-2-yl)benzoate and 2,5-Bis(trifluoromethyl)benzyl 4-(4-Oxo-4H-chromen-2-yl)benzoate

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Structured Abstract

Background: Flavonoids are a diverse group of naturally occurring compounds known for their wide range of medicinal benefits, including antioxidant, anti-inflammatory, and anticancer properties. Among them, flavones represent a key subclass that plays important roles in both plant physiology and human health. This study focuses on the synthesis of novel flavone derivatives that have not been previously reported. The significance of this research lies in the synthesis and structural characterization of these compounds using Infrared (IR) spectroscopy, Nuclear Magnetic Resonance (NMR), and Mass Spectrometry (MS).

Methods: The synthesis of the two flavone derivatives involved three key steps. First, chalcone acid was synthesized via Claisen–Schmidt condensation between 2'-hydroxyacetophenone and 4-carboxybenzaldehyde. The resulting chalcone acid then underwent oxidative cyclization with iodine under reflux conditions to form 4-(4-oxo-4H-chromen-2-yl)benzoic acid. This intermediate was further reacted with 1-bromoacetylpyrene to yield Flavone 1, identified as 2-oxo-2-(pyren-1-yl)ethyl 4-(4-oxo-4H-chromen-2-yl)benzoate. Flavone 2 was synthesized by esterification of the same benzoic acid intermediate with 2,5-bis(trifluoromethyl)benzyl bromide. The structures of both flavones were confirmed using IR spectroscopy, NMR spectroscopy, and mass spectrometry.

Results: Both flavone derivatives were successfully synthesized and characterized using IR, NMR, and mass spectrometry. The IR spectra of both compounds showed key absorption bands around 1720 cm⁻¹ (C=O stretch) and 1600 cm⁻¹ (aromatic C=C), indicating the presence of ester and flavone functional groups. In the ¹H and ¹³C NMR spectra, characteristic chemical shifts corresponding to aromatic protons, olefinic protons, and ester-linked methylene groups were observed, consistent with the proposed structures. Flavone 1 displayed additional aromatic signals corresponding to the pyrene ring, while flavone 2 showed signals corresponding to the trifluoromethyl-substituted benzyl group. Mass spectrometry further confirmed the molecular weights of both compounds, with molecular ion peaks matching the calculated m/z values.

Conclusion: Two novel flavone derivatives, 2-oxo-2-(pyren-1-yl)ethyl 4-(4-oxo-4H-chromen-2-yl)benzoate (Flavone 1) and 2,5-bis(trifluoromethyl)benzyl 4-(4-oxo-4H-chromen-2-yl)benzoate (Flavone 2), were successfully synthesized and characterized using IR, NMR, and mass spectrometry. The yields were 39.71% and 33.2%, respectively, confirming the success of the synthetic approach.

Keywords: Synthesis, Characterization, Flavones

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