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Synthesis And Characterization Of  
2-(Trifluoromethoxy) Benzyl 4-(4-Oxo-4H-Chromen-2-yl) Benzoate And  
2-Oxo-2-(2-Oxo-2H-Chromen-3-yl) Ethyl 4-(4-Oxo-4H-Chromen-2-yl) Benzoate

Nur Ellyia Nadzirah Raji<sup>e</sup><sup>a</sup>, Syahrul Imran Abu Bakar<sup>a\*</sup>**Structured Abstract**

**Background:** Natural products play an important role in drug discovery, offering therapeutic potential across multiple therapeutic areas. Flavonoids, a major class of natural compounds, possess diverse biological activities such as antioxidant, anti-inflammatory, and anticancer effects. However, limited natural abundance and complex structures challenge their development. Synthetic derivatives of flavonoids are being explored to enhance pharmacological properties. In this study, two novel flavone derivatives, 2-(trifluoromethoxy) benzyl 4-(4-oxo-4H-chromen-2-yl) benzoate (61) and 2-oxo-2-(2-oxo-2H-chromen-3-yl) ethyl 4-(4-oxo-4H-chromen-2-yl) benzoate (63) were synthesized and characterized. These compounds remain unexplored, and this research aims to investigate their synthesis and confirm their structure through NMR, MS and IR.

**Methods:** The synthesized compounds were prepared through a three-step reaction involving Claisen-Schmidt condensation, oxidative cyclization, and esterification. Reactions were monitored using thin-layer chromatography (TLC). Products were purified by recrystallization and filtration. Structural characterization was conducted using melting point determination, IR spectroscopy, NMR spectroscopy (<sup>1</sup>H and <sup>13</sup>C), and Mass Spectrometry. The synthesis involved DMSO as the solvent and potassium carbonate as the base. Each synthesized compound was confirmed through spectral data ensuring accurate identification and purity of the flavone-based derivatives.

**Results:** Both flavone derivatives were successfully synthesized and characterized using FTIR, NMR, and mass spectrometry. The FTIR spectra showed peaks around 1713 cm<sup>-1</sup> (C=O stretch of ester) and 1608 cm<sup>-1</sup> (aromatic C=C), confirming the presence of ester and flavone functional groups. <sup>1</sup>H NMR spectra displayed characteristic aromatic and methylene signals with splitting patterns confirming structural symmetry, substitution, and proton environments of both compounds. <sup>13</sup>C NMR spectra revealed distinct carbonyl, aromatic, and methylene signals for both compounds, confirming conjugated structures with overlapping carbon environments. Mass spectrometry confirmed both compounds' identities via matching [M+H]<sup>+</sup> peak at m/z 441.094 and fragment peaks at m/z 267.06 with calculated values.

**Conclusion:** In conclusion, the compounds (61) and (63) were synthesized with 19.75% and 21.05% yield, respectively. The low yields may be due to unoptimized purification, including product loss during aqueous precipitation, use of basic filtration without vacuum or fine filter paper, and lack of proper quenching agents. Their structures were confirmed by IR, NMR, and MS, supporting the successful synthesis and characterization of both target compounds.

**Keywords:** Flavones, NMR, LCMS, Synthesis, Characterization

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