

A Promising Chromone-Based Compounds in Drug Discovery for New Anti-Inflammatory and Anti-Cancer Drugs

Kamal Rullah¹*, Nur Farisya Shamsudin¹

¹ Drug Discovery and Synthetic Chemistry Research Group, Department of Pharmaceutical Chemistry, Kulliyyah of Pharmacy, International Islamic University Malaysia, Bandar Indera Mahkota, 25200 Kuantan, Pahang, Malaysia.

*Corresponding author. Email: <u>kamalrullah@iium.edu.my</u>

ABSTRACT

Chromone, a group of heterocyclic compounds, has been recognised as a privileged structure for new drug discovery and development. These scaffolds have exhibited extensive acceptability due to their drug-like properties and versatile binding properties. Among several approved anti-inflammatory and anti-cancer drugs, these scaffolds show high selectivity for certain specific targets. For this reason, a significantly increasing number of research groups are interested in developing new synthetic methods and evaluating biological properties. In this view, we will discuss some of the important discoveries of chromone-based compounds as anti-inflammatory and anti-cancer agents, such as 2-(3,4-dimethoxyphenyl)-3-(4-fluorophenyl)-6-methoxy-4H-chromen-4-one (KR-1401-KW) which was found to be significantly active in suppressing PGE2-associated inflammatory responses and 3-(4-(chloromethyl)phenyl)-2-(3,4-dimethoxyphenyl)-7-methoxy-4H-chromen-4-one which was displayed potential inhibitor of UNC-51-like kinase 1 (ULK1) (KR-2201-NF) modulates autophagy and induces apoptosis in colon cancer. Moreover, computational evidence, including docking and molecular dynamics (MD) simulations, makes the compounds promising candidates for new anti-inflammatory and anti-cancer drugs.

Keywords: chromone; anti-inflammation; anti-cancer; docking study; molecular dynamics (MD) simulations

Supporting Agencies: Source of research funding by the Ministry of Education (MOE) through the Fundamental Research Grant Scheme (FRGS/1/2022/STG04/UIAM/02/2) and the International Islamic University of Malaysia-IIUM through Research Management Centre Grant 2020 (RMCG20-008-0008).

Indexing: Pharmaceutical Chemistry

