Latin American Journal of Pharmacy
(formerly *Acta Farmacéutica Bonaerense)*
Lat. Am. J. Pharm. **37** (6): 1257-63 (2018)

Received: January 29, 2018
Revised version: May 4, 2018
Accepted: May 5, 2018

Novel 4-Hydroxycoumarin Derivatives: Anti-Cancer Effects on Human Oral Cancer Cells

Lin GAO [1], Shanshan LI [1], Jun GAO [2], Hongtao FENG [3] & Zhenhua DING [1] *

[1] *Department of Radiation Medicine, Guangdong Provincial Key Laboratory of Tropical Disease Research, School of Public Health, Southern Medical University, Guangzhou 510515, China*
[2] *Department of dermatology & STD, Liuzhou Worker's Hospital, Fourth Affiliated Hospital of Guangxi Medical University, Guangxi 545000, China*
[3] *Centre for Micro Nano Systems and Bionic Medicine, Shenzhen Institutes of Advanced Technology Chinese Academy of Sciences, Shenzhen 518055, China*

SUMMARY. The reaction of 4-hydroxycoumarin with aromatic aldehyde (or malononitrile) gave two kinds of 4-hydroxycoumarin derivatives (**1-8**) and their structures were characterized via IR, ^{1}H NMR, HRMS, and single crystal X-ray crystallography. The *in vitro* anticancer activity of the synthesized products was studied and evaluated, in which four human oral cancer cell liness (HB, CNE-1, SAS and HSQ-89) were used in the screening tests. The results showed that compared with compounds **5-8**, compounds **1-4** with intramolecular hydrogen bonds exerted rather potent activity. In addition, the relationship between activity and structure of compounds **1-4** was further investigated through molecular docking study.

RESUMEN. La reacción de la 4-hidroxicumarina con un aldehído aromático (o malononitrilo) dio dos tipos de derivados de 4-hidroxicumarina (**1-8**) y sus estructuras se caracterizaron mediante IR, ^{1}H NMR, HRMS y cristalografía de rayos X de cristal único. Se estudió y evaluó la actividad anticancerígena *in vitro* de los productos sintetizados, en la que se usaron cuatro líneas celulares de cáncer oral humano (HB, CNE-1, SAS y HSQ-89). Los resultados mostraron que, en comparación con los compuestos **5-8**, los compuestos **1-4** con enlaces de hidrógeno intramoleculares ejercían una actividad bastante más potente. Además, la relación entre la actividad y la estructura de los compuestos **1-4** se investigó a través del estudio de acoplamiento molecular.

KEY WORDS: 4-hydroxycoumarin, molecular docking, oral cancer cell, X-ray.

* Author to whom correspondence should be addressed. *E-mail:* dingzh@smu.edu.cn

ISSN 0326 2383 (printed ed.)
ISSN 2362-3853 (on line ed.)