

A New Organic Heterocycles Compound: Crystal Structure and Anti-Cancer Activity in Skin Cancer

Zhongzhao ZHANG¹, Jin ZHANG², & Yiqi DU^{3*}

¹ Department of Dermatology, The Second Affiliated Hospital of Guangzhou University of Chinese Medicine, Guangzhou, Guangdong, China

² Department of Dermatology, The 195 Hospital of Chinese People's Liberation Army, Xianning, Hubei, China

³ Department of Dermatology, San Shui Branch Foshan Hospital of TCM, Foshan, Guangdong, China

SUMMARY. The new heterocycles compound N-((3R,4R)-1-benzyl-4-methylpiperidin-3-yl)-N-methyl-7H-pyrrolo[2,3-d]pyrimidin-4-amine (**1**), designed using 4-chloro-7H-pyrrolo[2,3-d]pyrimidine (**2**) as start material, was successfully obtained via multiple synthesis route and finally characterized by IR, ¹H NMR, and single crystal X-ray crystallography. In addition, *in vitro* anticancer activity of compound **1** on three human skin cancer cell lines (A431, SK23 and HME1) was further determined.

RESUMEN. El nuevo compuesto heterocíclico N-((3R,4R)-1-bencil-4-metilpiperidin-3-il)-N-metil-7H-pirrol[2,3-d]pirimidin-4-amino (**1**), diseñado utilizando 4-cloro-7H-pirrol[2,3-d] pirimidina (**2**) como material de partida, se obtuvo con éxito por vía de síntesis múltiple y finalmente se caracterizó por IR, ¹H RMN y cristalografía de rayos X de cristal único. Además, se determinó adicionalmente la actividad anticancerígena *in vitro* del compuesto **1** en tres líneas celulares de cáncer de piel humano (A431, SK23 y HME1).

KEY WORDS: heterocycles, skin cancer, X-ray.

* Author to whom correspondence should be addressed. E-mail: yiqi_du666@yeah.net