

Crystal Structure and Anti-cancer Activity of (S)-3-[4-(2-chloro-5-iodobenzyl)phenoxy]tetrahydrofuran

Peng ZHANG, Zhi LI, Jiangtao LIU, Ruyi JIN, Xiaomei ZHAO & Hui GUO*

School of Pharmacy, Shaanxi University of Chinese Medicine,
Xiayang, Shaanxi, China

SUMMARY. The new heterocycles compound (S)-3-[4-(2-chloro-5-iodobenzyl)phenoxy]tetrahydrofuran (**1**), designed using 2-chloro-5-iodobenzoic acid (**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 cancer cells (A549, H1299 and PC9) was further determined, which suggested that compound **1** may be potential anticancer agent.

RESUMEN. El nuevo compuesto de heterociclo (S)-3-[4-(2-cloro-5-yodobencil)fenoxi]tetrahidrofurano (**1**), diseñado utilizando ácido 2-cloro-5-yodobenzoico (**2**) como material de partida, se obtuvo con éxito a través de ruta de síntesis múltiple y finalmente caracterizada por IR, ¹H NMR y cristalografía de rayos X de cristal único. Además, se determinó adicionalmente la actividad anticancerígena *in vitro* del compuesto **1** en tres células cancerosas humanas (A549, H1299 y PC9), lo que sugiere que el compuesto **1** puede ser un posible agente anticancerígeno.

KEY WORDS: anticancer activity, heterocycles, X-ray.

* Author to whom correspondence should be addressed. E-mail: hui_guo12@sina.com