Latin American Journal of Pharmacy
(formerly *Acta Farmacéutica Bonaerense)*
Lat. Am. J. Pharm. **37** (6): 1226-30 (2018)

Received: January 21, 2018
Revised version: May 2, 2018
Accepted: May 3, 2018

Comprehensive *In Vitro* and *In Silico* Analyses of Differences in Inhibitory Propertiesof Taxifolin for Mammalian and Mushroom Tyrosinases

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***SUMMARY*. This study aimed to investigate the inhibitory characteristics of taxifolin for tyrosinases using comprehensive *in vitro* and *in silico* analyses. Taxifolin and arbutin inhibited 62.74 ± 3.35% and 63.19 ± 0.78%, respectively, of mammalian tyrosinase activity at 100 μM. At 50 μM, taxifolin and arbutin inhibited 48.96 ± 2.71% and 43.96 ± 2.26% of mammalian tyrosinase activity. The docked poses of inhibitors in the active site cavity showed characteristic metal geometry in both mushroom and mammalian tyrosinases. This difference between mushroom and mammalian tyrosinases was caused by differing copper geometries. In the case of taxifolin, 57.37 of docking score in the mushroom tyrosinase was decreased more to 52.71 in the mammalian. However, docking scores of arbutin were increased from 50.52 to 53.81 when the tyrosinase model was changed. These results suggest that tyrosinase inhibitors should be investigated with a suitable protein model for the development of biologically active compounds.**

RESUMEN. El objetivo de este estudio fue investigar las características inhibitorias de taxifolina para tirosinasas utilizando análisis exhaustivos *in vitro* e *in silico*. La taxifolina y la arbutina inhibieron 62.74 ± 3.35% y 63.19 ± 0.78%, respectivamente, de la actividad tirosinasa de los mamíferos a 100 μM. A 50 μM, la taxifolina y la arbutina inhibieron 48.96 ± 2.71% y 43.96 ± 2.26% de la actividad tirosinasa de mamíferos. Las posiciones acopladas de los inhibidores en la cavidad del sitio activo mostraron una geometría metálica característica tanto en tirosinasas de hongos como de mamíferos. Esta diferencia entre las tirosinasas de hongos y mamíferos fue causada por diferentes geometrías del cobre. En el caso de la taxifolina, 57.37 de la puntuación de atraque en la tirosinasa de hongos disminuyó a 52.71 en mamíferos. Sin embargo, los puntajes de atraque de arbutina aumentaron de 50.52 a 53.81 cuando se modificó el modelo de tirosinasa. Estos resultados sugieren que los inhibidores de tirosinasa deberían investigarse con un modelo de proteína adecuado para el desarrollo de compuestos biológicamente activos.

KEY WORDS: metal ion interaction, molecular modeling, taxifolin, tyrosinase

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