

XANTHINE OXIDASE INHIBITORY PROPERTIES AND *IN SILICO* STUDY OF THREE N-(α -BROMOACYL)- α -AMINO ESTERS

Žaklina Šmelcerović¹, Katarina Tomović², Denitsa Yancheva³,
Emiliya Cherneva⁴, Gordana Kocić⁵, Živomir Petronijević⁶

Three noncyclic N-(α -bromoacyl)- α -amino esters, methyl 2-(2-bromo-3-methylbutanamido)-pentanoate (**1**), methyl 2-(2-bromo-3-methylbutanamido)-2-phenylacetate (**2**) and methyl 2-(2-bromo-3-methylbutanamido)-3-phenylpropanoate (**3**), were assayed for inhibitory activity against commercial enzyme xanthine oxidase (XO) *in vitro* and XO in rat liver homogenate. The assayed compounds did not show any significant inhibitory effect against commercial XO, nor against rat liver XO, at the tested concentration (50 μ g/ml). The absence of significant XO inhibitory activity might be caused by basically noncyclic molecular structure of compounds **1-3**, what is in accordance with the presented proposal about depsipeptides that the cyclic structure is important and required for the biological activity. On the other hand, the favorable pharmacokinetic behavior and toxicological properties of the assayed esters, predicted by *in silico* study, may represent a beneficial prerequisite for their implementation in rational carrier-linked prodrug strategies and design. *Acta Medica Medianae* 2016;55(4):14-20.

Key words: N-(α -bromoacyl)- α -amino esters, xanthine oxidase inhibition, *in silico* study, prodrug