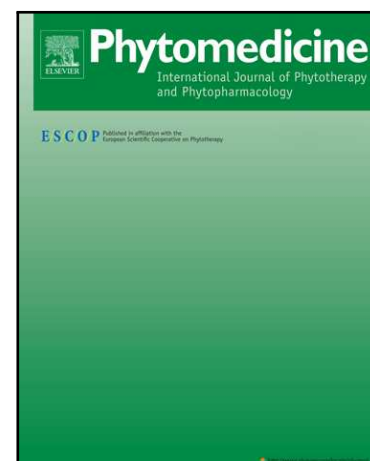


## Accepted Manuscript

Molecular modeling and in vitro approaches towards cholinesterase inhibitory effect of some natural xanthohumol, naringenin, and acyl phloroglucinol derivatives

Ilkay Erdogan Orhan , Dariusz Jedrejek , F. Sezer Senol ,  
Ramin Ekhteiari Salmas , Serdar Durdagi , Iwona Kowalska ,  
Lukasz Pecio , Wieslaw Oleszek

PII: S0944-7113(18)30040-0  
DOI: [10.1016/j.phymed.2018.03.009](https://doi.org/10.1016/j.phymed.2018.03.009)  
Reference: PHYMED 52383



To appear in: *Phytomedicine*

Received date: 27 October 2017  
Revised date: 7 January 2018  
Accepted date: 4 March 2018

Please cite this article as: Ilkay Erdogan Orhan , Dariusz Jedrejek , F. Sezer Senol , Ramin Ekhteiari Salmas , Serdar Durdagi , Iwona Kowalska , Lukasz Pecio , Wieslaw Oleszek , Molecular modeling and in vitro approaches towards cholinesterase inhibitory effect of some natural xanthohumol, naringenin, and acyl phloroglucinol derivatives, *Phytomedicine* (2018), doi: [10.1016/j.phymed.2018.03.009](https://doi.org/10.1016/j.phymed.2018.03.009)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

# Molecular modeling and *in vitro* approaches towards cholinesterase inhibitory effect of some natural xanthohumol, naringenin, and acyl phloroglucinol derivatives

Ilkay Erdogan Orhan<sup>a,\*</sup>, Dariusz Jedrejek<sup>b</sup>, F. Sezer Senol<sup>a</sup>, Ramin Ekhteiari Salmas<sup>c</sup>, Serdar Durdagi<sup>c</sup>, Iwona Kowalska<sup>b</sup>, Lukasz Pecio<sup>b</sup>, Wieslaw Oleszek<sup>b</sup>

<sup>a</sup>Department of Pharmacognosy, Faculty of Pharmacy, Gazi University, 06330 Ankara, Turkey

<sup>b</sup>Institute of Soil Science and Plant Cultivation, State Research Institute, Czartoryskich 8, 24-100 Pulawy, Poland

<sup>c</sup>Computational Biology and Molecular Simulations Laboratory, Department of Biophysics, School of Medicine, Bahcesehir University, 34349 Istanbul, Turkey

\*Corresponding author:

Ilkay Erdogan Orhan, Ph.D.

E-mail address: (iorhan@gazi.edu.tr)

## ABSTRACT

**Background:** Many natural products, particularly phenolic compounds, have been reported to have a strong inhibition against acetylcholinesterase (AChE) and butyrylcholinesterase (BChE), the key enzymes in the pathology of Alzheimer's disease (AD).

**Hypothesis:** Therefore, we hypothesized that some xanthohumol, naringenin, and acyl phloroglucinol derivatives (**1-14**) isolated from *Humulus lupulus* L. (hops) may have an inhibitory potential against AChE and BChE.

**Methods:** Inhibitory potential of compounds **1-14** were tested against AChE and BChE using ELISA microtiter assay. Different molecular docking simulations, including IFD and GOLD protocols, were implemented to verify the interactions between the ligands and the active site amino acids and also their binding energies inside the catalytic crevices of AChE and BChE. ADME/Tox analysis were used to determine pharmacological activities of the compounds.

Download English Version:

<https://daneshyari.com/en/article/8518424>

Download Persian Version:

<https://daneshyari.com/article/8518424>

[Daneshyari.com](https://daneshyari.com)